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=> fil hcapl
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FILE COVERS 1907 - 15 May 2003  VOL 138 ISS 20
FILE LAST UPDATED: 14 May 2003  (20030514/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d que l21; d que l19; d que l25; d que l32; d que l39; d que l56

L3       219941 SEA FILE=HCAPLUS ABB=ON  OXIDATION+OLD,NT/CT
L4        72723 SEA FILE=HCAPLUS ABB=ON  OXIDATION CATALYSTS+NT/CT
L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL -Role CAT = catalyst use
L18         511 SEA FILE=HCAPLUS ABB=ON  L17 AND (L3 OR L4)
L20       13065 SEA FILE=HCAPLUS ABB=ON  APROTIC
L21           4 SEA FILE=HCAPLUS ABB=ON  L18 AND L20

L3       219941 SEA FILE=HCAPLUS ABB=ON  OXIDATION+OLD,NT/CT
L4        72723 SEA FILE=HCAPLUS ABB=ON  OXIDATION CATALYSTS+NT/CT
L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L6            1 SEA FILE=REGISTRY ABB=ON  75-89-8
L7            1 SEA FILE=REGISTRY ABB=ON  920-66-1
L8           34 SEA FILE=REGISTRY ABB=ON  (536-80-1/BI OR 75-89-8/BI OR
                 920-66-1/BI OR 1088-11-5/BI OR 1119-94-4/BI OR 127256-73-9/BI
                 OR 13002-65-8/BI OR 1515-14-6/BI OR 179024-48-7/BI OR 20927-53-
                 1/BI OR 245329-97-9/BI OR 288-32-4/BI OR 2888-64-4/BI OR
                 363608-72-4/BI OR 363608-73-5/BI OR 363608-74-6/BI OR 363608-75
                 -7/BI OR 363608-76-8/BI OR 363608-77-9/BI OR 364043-33-4/BI OR
                 371-62-0/BI OR 375-01-9/BI OR 422-05-9/BI OR 439-14-5/BI OR
                 4797-43-7/BI OR 604-75-1/BI OR 631-61-8/BI OR 7722-84-1/BI OR
                 79968-43-7/BI OR 846-50-4/BI OR 91463-17-1/BI OR 937-14-4/BI
                 OR 963-39-3/BI OR 98-08-8/BI)
L9            9 SEA FILE=REGISTRY ABB=ON  L8 AND F/ELS
L10           1 SEA FILE=REGISTRY ABB=ON  C4H4F6O/MF AND L9
L12           1 SEA FILE=REGISTRY ABB=ON  L9 AND BENZENE
L13        3273 SEA FILE=HCAPLUS ABB=ON  L6
L14        1286 SEA FILE=HCAPLUS ABB=ON  L7
L15          92 SEA FILE=HCAPLUS ABB=ON  L10
L16        1212 SEA FILE=HCAPLUS ABB=ON  L12
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL
L18         511 SEA FILE=HCAPLUS ABB=ON  L17 AND (L3 OR L4)
L19           1 SEA FILE=HCAPLUS ABB=ON  (L13 OR L14 OR L15 OR L16) AND L18
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L4 and L5 L17

Oxidation Catal and Metallo (L) cat Role

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L3       219941 SEA FILE=HCAPLUS ABB=ON  OXIDATION+OLD,NT/CT
L4        72723 SEA FILE=HCAPLUS ABB=ON  OXIDATION CATALYSTS+NT/CT
L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL
L18         511 SEA FILE=HCAPLUS ABB=ON  L17 AND (L3 OR L4)
L23        8464 SEA FILE=HCAPLUS ABB=ON  PHASE TRANSFER CATALYSTS+OLD,RTCS/CT
L25           4 SEA FILE=HCAPLUS ABB=ON  L18 AND L23


L3       219941 SEA FILE=HCAPLUS ABB=ON  OXIDATION+OLD,NT/CT
L4        72723 SEA FILE=HCAPLUS ABB=ON  OXIDATION CATALYSTS+NT/CT
L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL
L18         511 SEA FILE=HCAPLUS ABB=ON  L17 AND (L3 OR L4)
L26           1 SEA FILE=REGISTRY ABB=ON  DICHLOROMETHANE/CN
L27           1 SEA FILE=REGISTRY ABB=ON  DICHLOROETHANE/CN
L28           3 SEA FILE=REGISTRY ABB=ON  TRICHLOROETHANE/CN
L29       31418 SEA FILE=HCAPLUS ABB=ON  (L26 OR L27 OR L28)
L30         507 SEA FILE=HCAPLUS ABB=ON  L18 NOT L29
L31       36649 SEA FILE=HCAPLUS ABB=ON  SOLVENTS/CT
L32           3 SEA FILE=HCAPLUS ABB=ON  L30 AND L31


L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL
L26           1 SEA FILE=REGISTRY ABB=ON  DICHLOROMETHANE/CN
L27           1 SEA FILE=REGISTRY ABB=ON  DICHLOROETHANE/CN
L28           3 SEA FILE=REGISTRY ABB=ON  TRICHLOROETHANE/CN
L29       31418 SEA FILE=HCAPLUS ABB=ON  (L26 OR L27 OR L28)
L37        5128 SEA FILE=HCAPLUS ABB=ON  (OXIDATION# OR OXIDN#)/OBI(1W)ORG?
L39           5 SEA FILE=HCAPLUS ABB=ON  L17 AND L37 NOT L29


L3       219941 SEA FILE=HCAPLUS ABB=ON  OXIDATION+OLD,NT/CT
L4        72723 SEA FILE=HCAPLUS ABB=ON  OXIDATION CATALYSTS+NT/CT
L5        60005 SEA FILE=HCAPLUS ABB=ON  METALLOPORPHYRINS+OLD,NT/CT
L17        1054 SEA FILE=HCAPLUS ABB=ON  L5(L)CAT/RL
L26           1 SEA FILE=REGISTRY ABB=ON  DICHLOROMETHANE/CN
L27           1 SEA FILE=REGISTRY ABB=ON  DICHLOROETHANE/CN
L28           3 SEA FILE=REGISTRY ABB=ON  TRICHLOROETHANE/CN
L29       31418 SEA FILE=HCAPLUS ABB=ON  (L26 OR L27 OR L28)
L52       12593 SEA FILE=HCAPLUS ABB=ON  HYDROCARBONS, REACTIONS/CT
L53        2765 SEA FILE=HCAPLUS ABB=ON  L52(L)OXID?
L56          23 SEA FILE=HCAPLUS ABB=ON  L17 AND (L3 OR L4) AND L53 NOT L29

=> s l21 or l19 or l25 or l32 or l39 or l56

L57          35 L21 OR L19 OR L25 OR L32 OR L39 OR L56

=> fil uspatf; d que l48

FILE 'USPATFULL' ENTERED AT 11:35:45 ON 15 MAY 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 13 May 2003 (20030513/PD)
FILE LAST UPDATED: 13 May 2003 (20030513/ED)
HIGHEST GRANTED PATENT NUMBER: US6564383
HIGHEST APPLICATION PUBLICATION NUMBER: US2003088899
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CA INDEXING IS CURRENT THROUGH 13 May 2003 (20030513/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 13 May 2003 (20030513/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2003
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2003

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
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>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

L45 97 SEA FILE=USPATFULL ABB=ON METALLOPORPHYRINS/CT
L46 12 SEA FILE=USPATFULL ABB=ON CATALY?/IT (L)L45
L47 682015 SEA FILE=USPATFULL ABB=ON OXID? OR OXID?/IT
L48 12 SEA FILE=USPATFULL ABB=ON L46 AND L47

=> dup rem l57,l48
FILE 'HCAPLUS' ENTERED AT 11:35:55 ON 15 MAY 2003
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FILE 'USPATFULL' ENTERED AT 11:35:55 ON 15 MAY 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L57
PROCESSING COMPLETED FOR L48
L58 47 DUP REM L57 L48 (0 DUPLICATES REMOVED)
ANSWERS '1-35' FROM FILE HCAPLUS
ANSWERS '36-47' FROM FILE USPATFULL

=> d ibib ab hitrn 1-47

L58 ANSWER 1 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2003:336636 HCAPLUS
DOCUMENT NUMBER: 138:309859
TITLE: Catalytic oxidations using ruthenium porphyrins
AUTHOR(S): Ezhova, Maria B.; James, Brian R.
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Catalysis by Metal Complexes (2003), 26(Advances in Catalytic Activation of Dioxygen by Metal Complexes), 1-77
CODEN: CMCOES; ISSN: 0920-4652
PUBLISHER: Kluwer Academic Publishers

Searched by Barb O'Bryen, STIC 308-4291

DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review; the major goal of the Chapter is to review developments in the use of Ru-porphyrin complexes as homogeneous (or matrix-supported) catalysts for oxygenation and oxidn. processes. The subject was given impetus with the discovery of a remarkable reaction in which a Ru(II) porphyrin complex reacted with O2 to give a trans-dioxo-Ru(VI) species. Such species, which can be formed from a wide range of O-atom donors, were shown subsequently to be capable of acting as a bis(monooxygenase) in transferring both the coordinated oxo ligands (as O-atoms) to olefinic substrates, satd. hydrocarbons, phosphines, and thioethers, and the processes become catalytic in the presence of excess of the O-atom donor. Further, the dioxo species can also exhibit oxidase-like activity, and effect stoichiometric or catalytic oxidative-dehydrogenation of phenols, alkoxyarenes, alcs., and amines. Use of chiral porphyrins has led to catalytic, asym. epoxidn. and hydroxylations, even though radical intermediates are invoked, as well as oxygenation of racemic substrates (phosphines and more interestingly tertiary alkanes) to yield chiral products by kinetic resoln. processes. The reaction mechanisms invoked range from genuine O-atom transfer (from RuVI, RuV, or RuIV species, where the disproportionation reaction [2 O=RuIV .dblharw. RuII + O=RuVI=O] is important), to free-radical induced processes, particularly when the porphyrin ligands are extensively halogenated, as Ru complexes generally of such porphyrins are extremely active in radical-type decompn. of hydroperoxides, often present as trace impurities in hydrocarbon substrates.
REFERENCE COUNT: 281 THERE ARE 281 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 2 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:123801 HCAPLUS
DOCUMENT NUMBER: 136:294443
TITLE: CO2-Expanded Solvents: Unique and Versatile Media for Performing Homogeneous Catalytic Oxidations
AUTHOR(S): Wei, Ming; Musie, Ghezai T.; Busch, Daryle H.; Subramaniam, Bala
CORPORATE SOURCE: Department of Chemical and Petroleum Engineering and Department of Chemistry, University of Kansas, Lawrence, KS, 66045-2223, USA
SOURCE: Journal of the American Chemical Society (2002), 124(11), 2513-2517
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The work summarized here demonstrates a new concept for exploiting dense phase CO2, media considered to be green solvents, for homogeneous catalytic oxidn. reactions. According to this concept, the conventional org. solvent medium used in catalytic chem. reactions is replaced substantially (up to 80 vol.%) by CO2, at moderate pressures (tens of bars), to create a continuum of CO2-expanded solvent media. A particular benefit is found for oxidn. catalysis; the presence of CO2 in the mixed medium increases the O2 soly. by .apprx.100 times compared to that in the neat org. solvent while the retained org. solvent serves an essential role by solubilizing the transition metal catalyst. CO2-expanded solvents provide optimal properties for maximizing oxidn. rates that are typically 1-2 orders of magnitude greater than those obtained with either the neat org. solvent or supercrit. CO2 as the reaction medium. These advantages are demonstrated with examples of homogeneous oxidns. of a substituted phenol and of cyclohexene by mol. O2 using transition metal catalysts, Co Schiff-base and Fe porphyrin complexes, resp., in CO2-expanded CH3CN.
IT **16456-81-8**

RL: **CAT (Catalyst use)**; CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(CO2-expanded solvents as unique and versatile media for performing homogeneous catalytic oxidns.)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 3 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:675277 HCAPLUS
DOCUMENT NUMBER: 138:153305
TITLE: Remarkable solvent effect on the yield and specificity of oxidation of naphthalene catalyzed by iron(III) porphyrins
AUTHOR(S): Khavasi, Hamid Reza; Hosseiny Davarani, S. Saeed; Safari, Nasser
CORPORATE SOURCE: Chemistry Department, Shahid Beheshti University, Evin, Tehran, 19839, Iran
SOURCE: Journal of Molecular Catalysis A: Chemical (2002), 188(1-2), 115-122
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:153305
AB Oxidn. of naphthalene was performed with tetrakis(pentafluorophenyl)porphyrin iron(III) chloride (F20TPPFeIIICl) or tetrakis(2,6-dichlorophenyl)porphyrin iron(III) chloride (TDCPPFeIIICl) or tetramesitylporphyrin iron(III) chloride (TMPFeIIICl) as catalyst and m-chloroperbenzoic acid or pentafluoroiodosylbenzene or tert-Bu hydroperoxide as oxidant in different media in the presence of imidazole as cocatalyst. In an **aprotic** solvent (CH3CN:CH2Cl2 1:1) and in the presence of F20TPPFeIIICl, 1-naphthol, 2-naphthol and 1,4-naphthoquinone yields based on m-chloroperbenzoic acid oxidant were 77.7, 2.1 and 5.6%, resp. The best yield for 1,4-naphthoquinone occurred in methanol with F20TPPFeIIICl and was 52.8%. The effect of bases on the yield and specificity of the naphthalene oxidn. were studied. When imidazole was changed to pyridine in F20TPPFeIIICl, the yield of 1-naphthol decreased from 77.7 to 55.3%, whereas for TDCPPFeIIICl catalyst, the yield changed from 61.1 to 18.3%.
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 4 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:218837 HCAPLUS
DOCUMENT NUMBER: 137:5840
TITLE: Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons
AUTHOR(S): Avdeev, M. V.; Bagrii, E. I.; Maravin, G. B.; Korolev, Yu. M.
CORPORATE SOURCE: Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, 117912, Russia
SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2002), 43(1), 38-44
CODEN: KICAA8; ISSN: 0023-1584
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Conference proceedings. The oxidn. of cyclic hydrocarbons by potassium peroxymonosulfate catalyzed by the iron and manganese complexes of tetra-(4-N-butylpyridinium)porphyrin, tetraphenylporphyrin, and mixed porphyrins contg. Ph and butylpyridyl substituents was studied in an aq. acetonitrile medium. The test catalysts were dissolved in the reaction

medium or adsorbed on layered aluminosilicates. It was found that the immobilization of metal complexes on layered aluminosilicates, as well as the bromination of porphyrins, decreased the activity of catalysts in a no. of cases, although it improved their stability. The addn. of pyridine in an equimolar amt. with respect to metal complexes to the reaction mixt. increased the activity of dissolved manganese complexes. An increase in the no. of butylpyridyl meso-substituents in a porphyrin mol. improved the catalytic activity of a metal complex.

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 5 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:115086 HCAPLUS
DOCUMENT NUMBER: 134:178573
TITLE: Process for the metalloporphyrin catalyzed **oxidation** of **organic** compounds
INVENTOR(S): Bernardelli, Patrick
PATENT ASSIGNEE(S): Warner Lambert Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809

PRIORITY APPLN. INFO.: US 1999-148079P P 19990810
US 1999-150101P P 19990820
WO 2000-EP7726 W 20000809

OTHER SOURCE(S): CASREACT 134:178573

AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, **aprotic**, polyhalogenated solvent (benzotrifluoride). Oxidn. of diazepam is conducted to mimic oxidn. (metab.) in biol. systems. The products of the oxidn. of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert **aprotic** solvent shows improved oxidn. yields when compared to prior art (e.g., CH3CN-CH2Cl2-water mixts.).

IT **920-66-1**, 1,1,1,3,3,3-Hexafluoro-2-propanol
RL: CAT (Catalyst use); USES (Uses)
(co-solvent; process for metalloporphyrin-catalyzed **oxidn.** of **org.** compds.)

IT **75-89-8**, 2,2,2-Trifluoroethanol
RL: NUU (Other use, unclassified); USES (Uses)

(co-solvent; process for metalloporphyrin-catalyzed **oxidn.** of **org.** compds.)

IT **98-08-8**, Benzotrifluoride
RL: NUU (Other use, unclassified); USES (Uses)
(process for metalloporphyrin-catalyzed **oxidn.** of **org**. compds.)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 6 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:694140 HCAPLUS
DOCUMENT NUMBER: 136:166904
TITLE: Iron polynitroporphyrins bearing up to eight .beta.-nitro groups as interesting new catalysts for H2O2-dependent hydrocarbon oxidation: unusual regioselectivity in hydroxylation of alkoxybenzenes
AUTHOR(S): Bartoli, Jean-Francois; Le Barch, Karine; Palacio, Magali; Battioni, Pierrette; Mansuy, Daniel
CORPORATE SOURCE: UMR 8601, Universite Paris V, Paris, 75270, Fr.
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (18), 1718-1719
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of iron porphyrins bearing one to eight .beta.-nitro substituents were synthesized and evaluated as catalysts for hydrocarbon oxidn. with H2O2. Iron porphyrins bearing five or six .beta.-nitro groups were the best catalysts for cyclooctene epoxidn. and adamantane or anisole hydroxylation without need of a cocatalyst. Very different regioselectivities were obsd. with either H2O2 or PhIO as oxidants, as shown by an unusual ortho-hydroxylation of alkoxybenzenes highly favored in the H2O2-dependent oxidns.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 7 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:344513 HCAPLUS
DOCUMENT NUMBER: 134:326198
TITLE: Catalytic oxidation of alkanes or cycloalkanes using metalloporphyrins
INVENTOR(S): Guo, Cancheng; Liu, Qiang; Zhang, Xiaobing
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 8 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1269343	A	20001011	CN 2000-113225	20000117

PRIORITY APPLN. INFO.: CN 2000-113225 20000117
OTHER SOURCE(S): CASREACT 134:326198; MARPAT 134:326198

AB Alkanes or cycloalkanes are oxidized at 1 atm air at 25-120.degree. in the presence of 40-200 ppm metalloporphyrin catalyst and catalyst adjuvant. The mole ratio of metalloporphyrin to catalyst adjuvant is 1:3-5. The metalloporphyrin or its oxide is [5,10,15,20-tetra(4- R1-3-R2-2-R3-phenyl)porphyrin]MX or [5,10,15,20-tetra(4-R1- 3-R2-2-R3-phenyl)porphyrin]M1 [5,10,15,20-tetra(4-R1-3- R2-2-R3-phenyl)porphyrin]M2 oxide (M, M1, and/or M2 = transition metal or lanthanide; and R1, R2, and/or R3 = H, alkyl, alkoxy, halo, amino, alkylamino, glycosyl, or

cyclodextrin group; and X = acetate, acetoacetonato, halide, or other acid group-type anion). The carrier for metalloporphyrin catalyst is silica gel, mol. sieve, Al2O3, zeolite, sepiolite, porous ceramics, polyvinyl chloride, polyvinyl perchloride, or polystyrene, etc. The catalyst adjuvant is salt or oxide of Cu, Zn, Fe, Co, Mn, Cr, or Ni, etc.

L58 ANSWER 8 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:442953 HCAPLUS
DOCUMENT NUMBER: 133:176887
TITLE: Evidence for the Participation of Two Distinct Reactive Intermediates in Iron(III) Porphyrin Complex-Catalyzed Epoxidation Reactions
AUTHOR(S): Nam, Wonwoo; Lim, Mi Hee; Lee, Ha Jin; Kim, Cheal
CORPORATE SOURCE: Department of Chemistry and Division of Molecular Life Sciences, Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Journal of the American Chemical Society (2000), 122(28), 6641-6647
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have studied the competitive epoxidns. of olefins with cis- and trans-stilbenes and with cyclooctene and trans-stilbene in iron porphyrin complex-catalyzed epoxidn. reactions by H2O2, tert-Bu hydroperoxide (t-BuOOH), and m-chloroperoxybenzoic acid (m-CPBA) in protic solvent (i.e., a solvent mixt. of CH3OH and CH2Cl2) and **aprotic** solvent (i.e., a solvent mixt. of CH3CN and CH2Cl2) at room temp. under catalytic reaction conditions. The competitive epoxidns. were also carried out with in situ generated high-valent iron(IV) oxo porphyrin cation radical complexes in **aprotic** solvent under stoichiometric reaction conditions. By detg. the ratios of epoxide products formed in the competitive epoxidns., we were able to conclude unambiguously that the reactive species generated in protic solvent are high-valent iron(IV) oxo porphyrin cation radical complexes 3 [FeIV:O-Porp.bul.+] and the intermediates formed in **aprotic** solvent are oxidant-iron porphyrin intermediates 2 [e.g., FeIIIOOH-Porp]. A protic solvent such as methanol is proposed to function as a general-acid catalyst, thereby increasing the rate of O-O bond cleavage of 2 to form 3. In the absence of general-acid catalysis such as in **aprotic** solvent, the rate of O-O bond cleavage of 2 is relatively slow and 2 transfers its oxygen to olefins prior to the formation of 3. To further examine the effect of the general-acid catalysis on the nature of epoxidizing intermediates, we carried out competitive epoxidns. in the solvent mixts. of alc./CH2Cl2 using alcs. of varying pKa values and in the presence of an acid (i.e., HClO4) in **aprotic** solvent. The product ratios were found to vary depending on the strength of the solvent acidity, demonstrating that the reaction of 2 with olefin competes with the O-O bond cleavage of 2 that leads to the formation of 3. We also reported for the first time that a high-valent iron(IV) oxo porphyrin cation radical intermediate contg. electron-deficient porphyrin ligand shows an unexpected preference for trans-stilbene over cis-stilbene in the competitive epoxidns. of cis- and trans-stilbenes.
REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 9 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:735661 HCAPLUS
DOCUMENT NUMBER: 134:91666
TITLE: Metalloporphyrin catalytic oxidations of hydrocarbons by H2O2
AUTHOR(S): Rocha Gonsalves, Antonio M. d'A.; Serra, Armenio C.
CORPORATE SOURCE: Departamento de Quimica, Universidade de Coimbra,

Coimbra, P-3049, Port.
SOURCE: Journal of Porphyrins and Phthalocyanines (2000), 4(6), 598-603
CODEN: JPPHFZ; ISSN: 1088-4246
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The metalloporphyrin catalytic oxidn. of hydrocarbons using dil. hydrogen peroxide as oxygen donor with a two-phase system in the presence of an excess of benzoic acid is studied. Porphyrins derived from meso-tetrakis(2,6-dichlorophenyl)porphyrin and bearing sulfonamide substituents at .beta. or meso positions and halogens at .beta. positions were used. The system allowed for very efficient catalytic epoxidns. and hydroxylations of hydrocarbons. It is proved that the excess of benzoic acid is crit. to the catalyst efficiency and stability. The role of the lipophilic acid in this system is discussed.
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 10 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:273368 HCAPLUS
DOCUMENT NUMBER: 133:22890
TITLE: Synthesis and characterization of zeolite-encapsulated metalloporphyrins
AUTHOR(S): Nakagaki, S.; Xavier, C. R.; Wosniak, A. J.; Mangrich, A. S.; Wypych, F.; Cantao, M. P.; Denicolo, I.; Kubota, L. T.
CORPORATE SOURCE: Departamento de Quimica, Universidade Federal do Parana, Curitiba, Brazil
SOURCE: Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2000), 168(3), 261-276
CODEN: CPEAEH; ISSN: 0927-7757
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Metalloporphyrins of FeIII and CuII were prepd. inside the large pores of the zeolite NaY by a process of sequential introduction of components followed by assembly inside the void space of the zeolite. The appropriate process chosen for the porphyrin synthesis was using the propionic acid solvent for reaction between pyrrole and benzaldehyde and this solvent was not destructive for zeolite. The powder X-ray diffraction data confirmed that the crystallinity of the zeolite was maintained. The resulting materials were purified by Soxhlet extractor. The zeolite-included metalloporphyrins were identified for studies using UV-Vis, FTIR and EPR Spectroscopy, CA (chem. anal.), AAS (at. absorption spectroscopy), TG/DSC, XRD, SEM and 13C-NMR techniques. The catalytic activity of these products was examd. and the catalyst showed to be a promising catalytic system to aliph. hydrocarbon oxidn. reactions.
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 11 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:179461 HCAPLUS
DOCUMENT NUMBER: 132:278747
TITLE: Study on catalytic activation of dioxygen by polymer quasi-porphyrin complexes
AUTHOR(S): Wang, Rong-Min; Wang, Yun-Pu; Lei, Zi-Qiang
CORPORATE SOURCE: Chemistry & Chemical Engineering College, Northwest Normal University, Lanzhou, 730070, Peop. Rep. China
SOURCE: Xibei Shifan Daxue Xuebao, Ziran Kexueban (2000), 36(1), 100-103
CODEN: XDXKEH; ISSN: 1001-988X
PUBLISHER: Xibei Shifan Daxue

DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB A review with 21 refs. The development of efficient catalysts for the selective oxidn. of hydrocarbons in presence of mol. oxygen under mild condition has remained a difficult challenge. Much attention has been paid to the construction. of the active center - the quasi-porphyrin complex - and its polymer surroundings for mimicing the structure and properties of enzyme. We have used polymer-supported porphyrin and Schiff base complexes. They show higher activities in oxidn. of alkylbenzene, cyclohexene and long-chain linear aliph. olefins.

L58 ANSWER 12 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:445418 HCAPLUS
DOCUMENT NUMBER: 131:144244
TITLE: Catalysis of hydrocarbon oxidation by polyhalogenated ruthenium porphyrins and studies on the origins of enantioselectivity in metalloporphyrin catalyzed olefin epoxidations
AUTHOR(S): Shalyaev, Kirill V.
CORPORATE SOURCE: Princeton Univ., Princeton, NJ, USA
SOURCE: (1998) 201 pp. Avail.: UMI, Order No. DA9920463 From: Diss. Abstr. Int., B 1999, 60(2), 643
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable

L58 ANSWER 13 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:93389 HCAPLUS
DOCUMENT NUMBER: 128:180083
TITLE: Rapid catalytic oxygenation of hydrocarbons with perhalogenated ruthenium porphyrin complexes
AUTHOR(S): Groves, John T.; Shalyaev, Kirill V.; Bonchio, Marcella; Carofiglio, Tommaso
CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA
SOURCE: Studies in Surface Science and Catalysis (1997), 110(3rd World Congress on Oxidation Catalysis, 1997), 865-872
CODEN: SSCTDM; ISSN: 0167-2991
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Conference proceedings. Perhalogenated ruthenium porphyrins were found to be efficient catalysts for the oxygenation of hydrocarbons including secondary alkanes and benzene in the presence of 2,6-dichloropyridine N-oxide under mild conditions in **aprotic** media. Up to 15,000 turnovers and rates of 800 TO/min were obtained. A mechanism where Ru(III) - Ru(V) intermediates play an important role is proposed and discussed.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L58 ANSWER 14 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:386113 HCAPLUS
DOCUMENT NUMBER: 127:105856
TITLE: Biomimetic **oxidation** of **organic** substrates by chemical models of cytochrome P-450 and related heme monooxygenases
AUTHOR(S): Chauhan, S. M. S.
CORPORATE SOURCE: Department of Chemistry, University of Delhi, Delhi, 110 007, India
SOURCE: Journal of the Indian Chemical Society (1996), 73(12), 637-645

Searched by Barb O'Bryen, STIC 308-4291

CODEN: JICSAH; ISSN: 0019-4522
PUBLISHER: Indian Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 72 refs. Cytochromes P 450 are membrane-bound heme monooxygenases that catalyze the monooxygenation of a wide range of org. substrates by utilization of dioxygen and NADPH or NADH as reducing agents. The development of chem. models for cytochromes P 450 has been initiated to understand the mol. mechanisms of different cytochromes P 450 and to develop suitable catalysts for selective and mild oxidn. in org. synthesis and oxidative metab. of drugs, agrochems., and xenobiotics. The synthesis of metalloporphyrins and chem. models for cytochrome P 450 and demonstration of their biomimetic activities in oxidizing org. substrates is examd.

L58 ANSWER 15 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:680698 HCAPLUS
DOCUMENT NUMBER: 126:59546
TITLE: Aerobic oxidation of hydrocarbons catalyzed by electronegative iron salen complexes
AUTHOR(S): Boettcher, Arnd; Grinstaff, Mark W.; Labinger, Jay A.; Gray, Harry B.
CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 191-200
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A no. of salen derivs. bearing electroneg. substituents and their corresponding iron(III) chloro complexes have been prepd. Several of the complexes catalyze aerobic oxidn. of cyclohexene, primarily to allylic oxidn. products. Evidence supports a radical chain autoxidn. mechanism, with the complex functioning to decomp. intermediate alkyl hydroperoxides. Activity is obsd. only for complexes with relatively high Fe(III/II) redn. potentials, but the incomplete correlation of activity with potential indicates that more subtle structural and electronic effects also play an important role in detg. the rates of the catalytic reactions.
IT **16456-81-8**
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(aerobic oxidn. of hydrocarbons catalyzed by electroneg. iron salen complexes)

L58 ANSWER 16 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:680700 HCAPLUS
DOCUMENT NUMBER: 126:103763
TITLE: Nonradical tetrabutylammonium monopersulfate oxidation of hydrocarbons catalyzed by [Mn3O4bipy4(H2O)2](ClO4)4
AUTHOR(S): Wessel, Jeremy; Crabtree, Robert H.
CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven, CT, 06520, USA
SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 13-22
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:103763
AB Tetrabutylammonium monopersulfate (2NBu4HSO5.cntdot.NBu4HSO4.cntdot.(NBu4)2SO4) is an effective primary oxidant with a high tendency to promote oxo

transfer rather than radical pathways in catalysis. Nonradical hydrocarbon oxidn. is seen with the complex [Mn3O4bipy4(H2O)2](ClO4)4 as catalyst as indicated by mechanistic studies; this contrasts with the radical pathways found for the same catalyst with t-BuOOH as the primary oxidant. The catalyst is robust, giving up to 15000 catalytic turnovers, and very efficient, the rate of 1-alkene epoxidn. being 4000 turnovers/h.

L58 ANSWER 17 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:103134 HCAPLUS
DOCUMENT NUMBER: 124:218485
TITLE: The mechanism of catalytic hydrocarbon oxidation by molecular oxygen and halogenated ruthenium and iron porphyrins
AUTHOR(S): Birnbaum, Eva Rachel
CORPORATE SOURCE: California Institute of Technology, Pasadena, CA, USA
SOURCE: (1995) 355 pp. Avail.: Univ. Microfilms Int., Order No. DA9601103
From: Diss. Abstr. Int., B 1995, 56(9), 4876
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable

L58 ANSWER 18 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:502796 HCAPLUS
DOCUMENT NUMBER: 123:82524
TITLE: The highly efficient oxidation of olefins, alcohols, sulfides and alkanes with heteroaromatic N-oxides catalyzed by ruthenium porphyrins
AUTHOR(S): Ohtake, Hiro; Higuchi, Tsunehiko; Hirobe, Masaaki
CORPORATE SOURCE: Faculty Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Heterocycles (1995), 40(2), 867-903
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:82524
AB The O atom transfer reactions from 2,6-disubstituted pyridine N-oxides to olefins, allyl or benzyl alcs. and sulfides were efficiently catalyzed by Ru porphyrins, and these substrates were converted into epoxides, aldehydes and sulfoxides, resp., with high selectivity. These oxidns. also proceeded using other heteroarom. N-oxides, such as pyrazine N-oxides, as oxidants. The catalytic activity of Ru porphyrin complexes was enhanced by the addn. of a small amt. of HCl or HBr. In the presence of these acids, the oxidns. of alkanes or aliph. alcs. with 2,6-dichloropyridine N-oxides were also efficiently catalyzed by Ru porphyrin complexes, and alcs. or ketones were afforded as oxidn. products with high selectivity. In the hydroxylation of adamantane, Ru porphyrins work very efficiently as catalysts, giving a turnover no. of up to 120,000. This system offers practical advantages, such as mild conditions, tractability of oxidants and easy overall procedures. In the case of the reactions with HCl or HBr, one possibility in the reaction mechanism is that the activity of Ru porphyrins is enhanced in part by the coordination of Cl- or Br- as axial ligands.
IT **14172-90-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(lack of catalysis in oxidn. of olefins and alcs. and alkanes and sulfides by heteroarom. N-oxides)

L58 ANSWER 19 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:952970 HCAPLUS
DOCUMENT NUMBER: 124:67840
TITLE: Synthesis and catalytic performance of polymer-supported metalloporphyrins bearing polyglycol

chains
AUTHOR(S): Yu, Xiaoqi; Wei, Tingxian; Lan, Zhongwei; You, Jingsong; Zhao, Huaming
CORPORATE SOURCE: Dep. Chem., Sichuan Univ., Chengdu, 610064, Peop. Rep. China
SOURCE: Fenzi Cuihua (1995), 9(4), 244-50
CODEN: FECUEN; ISSN: 1001-3555
PUBLISHER: Zhongguo Kexueyuan Lanzhou Huaxue Wuli Yanjiuso
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Synthesis and catalytic performance of polymer-supported metalloporphyrins bearing polyglycol chains in CH2Cl2/H2O two-phase system were studied. The influence of pH values, concn. of NaOCl, axial ligands and phase transfer catalysts on the epoxidn. of styrene catalyzed by those catalysts have also been investigated. The exptl. results show that manganese (III) porphyrins bound to chloromethylated polystyrene which bears some polyglycerol chains are efficient catalysts for the epoxidn. of styrene by sodium hypochloride. The introduction of polyglycol chain increases the amt. of oxidant in the org. phase by extg. -OCl from the aq. phase. Under these conditions, the anion -OCl assocd. with the polyglycol chain is extremely reactive as an oxidant. In all factors studied exptl., the influence of pH values in aq. soln. is the greatest.

L58 ANSWER 20 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:286499 HCAPLUS
DOCUMENT NUMBER: 122:94975
TITLE: Oxidation reactions of Mononuclear Manganese(III) Complexes
AUTHOR(S): Gangopadhyay, Sumana; Ali, Mahammad; Banerjee, Pradyot
CORPORATE SOURCE: Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032, India
SOURCE: Coordination Chemistry Reviews (1994), 135/136, 399-427
CODEN: CCHRAM; ISSN: 0010-8545
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review, with 73 refs., is given on the oxidn. reactions of various Mn(III) coordinated mols. The reactions are categorized primarily with respect to the type of Mn(III) complexes. Emphasis is given to the reactivity of the Mn(III) complexes derived from aminopolycarboxylic acids, acetylacetone, porphyrins, bipyridine, and pyrophosphoric acid with various org., inorg., and biochem. electron donors. Kinetic and mechanistic features assocd. with the interactions are highlighted and analyzed critically. The utility and scope of the catalytic oxidn. of hydrocarbons and secondary amines by Mn(III) porphyrins are discussed at length.

L58 ANSWER 21 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:535380 HCAPLUS
DOCUMENT NUMBER: 123:32378
TITLE: Metalloporphyrin-catalyzed oxidation of hydrocarbons with dioxygen
AUTHOR(S): Mlodnicka, Teresa
CORPORATE SOURCE: Institute Catalysis and Surface Chemistry, Polish Academy Sciences, Krakow, Pol.
SOURCE: Metalloporphyrins Catal. Oxid. (1994), 261-96.
Editor(s): Sheldon, Roger A. Dekker: New York, N. Y.
CODEN: 60SIAM
DOCUMENT TYPE: Conference; General Review
LANGUAGE: English
AB A review with 154 refs.

L58 ANSWER 22 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:76659 HCAPLUS
DOCUMENT NUMBER: 120:76659
TITLE: Catalytic oxidation of saturated and aromatic hydrocarbons by tert-butyl hydroperoxide in the presence of rare earth porphyrin complexes
AUTHOR(S): Vedernikov, A. N.; Kochnev, D. O.; Suslov, D. A.; Solomonov, B. N.
CORPORATE SOURCE: Kazan. Gos. Univ., Russia
SOURCE: Doklady Akademii Nauk (1993), 330(2), 200-3 [Chem.]
CODEN: DAKNEQ; ISSN: 0869-5652
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 120:76659
AB Oxidn. of hydrocarbons, such as cyclohexane, adamantane, and PhMe, by Me3COOH in C6H6 catalyzed by 15 title complexes was studied. The overall yield of products is linearly dependent on catalyst concn. in the oxidn. of hydrocarbons catalyzed by (meso-tetraphenylporphyrinato)lutetium(III) hydroxide. The porphyrin ligand is an essential part of the catalyst.

L58 ANSWER 23 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:650744 HCAPLUS
DOCUMENT NUMBER: 117:250744
TITLE: Selective oxygenation of hydrocarbons and sulfoxidation of thioethers by dioxygen with a Mn-porphyrin-based cytochrome P450 model system using zinc as electron donor
AUTHOR(S): Lu, W. Y.; Bartoli, J. F.; Battioni, P.; Mansuy, D.
CORPORATE SOURCE: Lab. Chim. Biochem. Pharmacol. Toxicol., Univ. Paris V, Paris, 75270, Fr.
SOURCE: New Journal of Chemistry (1992), 16(5), 621-8
CODEN: NJCHE5; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:250744
AB Cyclooctene epoxidn. by O2 occurs, with consumption of reducing equivs. from Zn and protons from acetic acid, in the presence of two catalysts, Mn(TPP)Cl (H2TPP = 5,10,15,20-tetraphenylporphyrin) and 1-methylimidazole (1-MeIm). A comparative study made on ten different Mn(III) or Fe(III) porphyrin catalysts, ten nitrogen base cocatalysts and various carboxylic acids showed that the most efficient system involves Mn(TPP)Cl, 1-MeIm and CH3COOH in addn. to O2 and Zn in a CH3CN:CH2Cl2 mixt. This system selectively epoxidizes 2-methylhept-2-ene, cyclohexene, (+)-limonene, cis-stilbene and .alpha.-ionone with yields based on Zn between 34 and 58% and rates between 1 and 3 turnovers per min. It also epoxidizes 1-nonene, a less reactive alkene, and oxidizes alkanes like cyclooctane, cyclohexane, adamantane, indan, tetralin and heptane to the corresponding alcs. and ketones, but with lower yields (between 1 and 36%). Thioethers are selectively oxidized to the corresponding sulfoxides with yields up to 68%. The system exhibits a stereochem. for cis- and trans-stilbene epoxidn., a regioselectivity for the oxidn. of cyclohexene, limonene and heptane, and a chemoselectivity for the oxidn. of a cyclooctene-cyclooctane mixt., almost identical to those of the Mn(TPP)Cl-PhIO-1-MeIm system. This indicates that the Mn(TPP)Cl-O2-Zn-AcOH-1-MeIm system involves a (1-MeIm)Mn(V):O active oxygen species. This system was successfully used for the conversion of .alpha.-ionone to the corresponding epoxides and allylic ketone and of di-Bu thioether to its sulfoxide with high yields and without any denaturation of the catalyst.
IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for epoxidn. of cyclooctene)

L58 ANSWER 24 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:351792 HCAPLUS
DOCUMENT NUMBER: 122:159793
TITLE: Selective **oxidations** in **organic** chemistry using biomimetic catalysts
AUTHOR(S): Mansuy, Daniel
CORPORATE SOURCE: Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques, Universite Rene Descartes, Paris, 75270/06, Fr.
SOURCE: New Aspects Org. Chem. II, Proc. Int. Kyoto Conf., 5th (1992), Meeting Date 1991, 477-97. Editor(s): Yoshida, Zen-ichi; Ohshiro, Yoshiki. Kodansha: Tokyo, Japan.
CODEN: 60UNAD
DOCUMENT TYPE: Conference
LANGUAGE: English
AB New selective oxidn. catalysts mimicking cytochrome P 450-dependent monooxygenases have been obtained by following three strategies. The first one was based on Fe(III) or Mn(III) porphyrins as homogeneous catalysts in the presence of an oxygen atom donor like PhIO or H2O2. Good results have been obtained for the hydroxylation of linear alkanes and the oxidn. of methoxyarenes to quinones by using iron porphyrins bearing electron-withdrawing substituents on the pyrrole .beta.-positions. The second strategy was to prep. supported catalysts by incorporation of a metalloporphyrin in a polymer mineral matrix (covalent binding or adsorption on silica, intercalation into layered clays...). The biotechnol. catalysts prepd. after the third strategy have been obtained by expression of the genes coding for different human liver cytochrome P 450 isoenzymes in yeast. The specific properties of these various catalysts are compared.

L58 ANSWER 25 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:83060 HCAPLUS
DOCUMENT NUMBER: 116:83060
TITLE: Biomimetic activation of the carbon-hydrogen bond. 2. Oxygenation of hydrocarbons with O2 catalyzed by porphyrin metal complexes in the presence of ferrocene as reducing agent
AUTHOR(S): Shul'pin, G. B.; Druzhinina, A. N.
CORPORATE SOURCE: Inst. Khim. Fiz. im. Semenova, Moscow, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1991), (12), 2739-44
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Oxidn. of cyclohexane in the presence of metalloporphyrins, ferrocene, and O2 afforded cyclohexanol and cyclohexanone in varying degrees after an induction time; use of non-metal-contg. tetraphenylporphyrin resulted in a prolonged induction time followed by rapid oxidn.; use of benzylferrocene resulted in selectivity for cyclohexanol in higher overall product yield, as well as diminished induction period. PhEt afforded 1-phenylethanol and acetophenone; styrene afforded PhCHO, and metal effects on the rate of metalloporphyrin-catalyzed prodn. of PhCHO were studied. The parameter .phi. representing relative reactivity of C-H bonds in PhEt vs. cyclohexane was a sensitive function of reducing agent for a given catalyst and nearly coincided with .phi. that characterized hydroxylation reactions with hydroxyl radical.
IT **14172-90-8 16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for hydrocarbon oxidn. with oxygen in presence of ferrocene-derived reducing agents, biomimetic)

L58 ANSWER 26 OF 47 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1991:655433 HCAPLUS
DOCUMENT NUMBER: 115:255433
TITLE: Catalysis by metal porphyrins of the oxidation of unsaturated hydrocarbons in the presence of inverse micelles
AUTHOR(S): Borovkova, S. Yu.; Solov'eva, A. B.; Genkin, M. V.; Davydov, R. M.
CORPORATE SOURCE: Inst. Khim. Fiz. im. Semenova, Moscow, USSR
SOURCE: Zhurnal Fizicheskoi Khimii (1991), 65(8), 2279-83
CODEN: ZFKHA9; ISSN: 0044-4537
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Inverse micelles [of CTAB and Na bis(2-ethylhexyl)sulfosuccinate] in org. solvent mixts. increased the rate of oxidn. of unsatd. hydrocarbons (cholesterol, anthracene) catalyzed by the metalloporphyrin (e.g., tetraphenylporphyrinatomagnesium chloride)-NaBH4-O2 system in a narrow range of concn.; product distributions varied little, if at all. The concn. range for surfactant acceleration of the oxidn. rate significantly exceeded the crit. micelle concn. (cmc) for each surfactant studied; moreover, at fixed surfactant concn. > cmc, the rate was extremal in metalloporphyrin concn. These observations were interpreted in terms of reagent partition between the org. and micellar phases, as well as isolation of the active system (consisting of metalloporphyrin, oxygen, and substrate) from cyclic hydroperoxides (which destroy the metalloporphyrin).

IT **14172-90-8 16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, in presence of inverse micelles, for oxidn. of unsatd. hydrocarbons)

L58 ANSWER 27 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:188007 HCAPLUS
DOCUMENT NUMBER: 114:188007
TITLE: Production of detergent range alcohols and ketones from alkanes using porphyrin catalysts
INVENTOR(S): Sanderson, John R.; Marquis, Edward T.; Payton, Howard F.
PATENT ASSIGNEE(S): Texaco Chemical Co., USA
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4978799	A	19901218	US 1989-428812	19891030
EP 426290	A2	19910508	EP 1990-310155	19900917
EP 426290	A3	19910925		
R: DE, FR, GB, IT				
JP 03169831	A2	19910723	JP 1990-290985	19901030

PRIORITY APPLN. INFO.:
US 1989-428701 19891030
US 1989-428703 19891030
US 1989-428812 19891030

AB The reaction of C10-18 alkanes with a hydroperoxide, esp. tert-BuOOH or cumene hydroperoxide (I), in the presence of a transition metal (esp. Fe, Mn, or Co) porphyrin catalyst gives alcs. and ketones with minimal formation of byproducts. A mixt. of dodecane 50.0, chloroferric phthalocyanine 0.10, and imidazole 0.07 g was treated slowly at 30.degree. with 80% I to give 5.02% dodecanones and 1.42% dodecanols.

IT **1643-19-2**, Tetrabutylammonium bromide **14172-90-8** **16456-81-8**

RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for oxidn. of alkanes to alcs. and ketones)

L58 ANSWER 28 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:197650 HCAPLUS
DOCUMENT NUMBER: 112:197650
TITLE: Metalloporphyrin-catalyzed oxidation of saturated hydrocarbons with sodium chlorite
AUTHOR(S): Collman, James P.; Tanaka, Hiroo; Hembre, Robert T.; Brauman, John I.
CORPORATE SOURCE: Dep. Chem., Stanford Univ., Stanford, CA, 94305-5080, USA
SOURCE: Journal of the American Chemical Society (1990), 112(9), 3689-90
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:197650
AB A remarkably efficient and active catalyst is formed when NaClO2, a manganese porphyrin, and an axial base such as 4-tert-butylpyridine are used in the oxidn. of satd. hydrocarbons. The unique reactivity of the chlorite-derived oxidant is contrasted with the active species formed by other shunt oxidants - in particular, hypochlorite. Mn(III)-porphyrin catalysis of chlorite disproportionation to chlorate and chloride is also reported.

L58 ANSWER 29 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:413600 HCAPLUS
DOCUMENT NUMBER: 113:13600
TITLE: Functionalization of saturated hydrocarbons. Part XV. Electrochemical oxidation of saturated hydrocarbons by the Gif-Orsay system
AUTHOR(S): Balavoine, G.; Barton, D. H. R.; Boivin, J.; Gref, A.; Hallery, I.; Ozbalik, N.; Pestana, J. A.; Riviere, H.
CORPORATE SOURCE: Inst. Chim. Mol. Orsay, Univ. Paris-Sud, Orsay, 91405, Fr.
SOURCE: New Journal of Chemistry (1990), 14, 175-83
CODEN: NJCHE5; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The various components of the Gif-Orsay system for selective oxidn. of satd. hydrocarbons and their interactions with each other were examd. by cyclic voltammetry. This study permitted to establish the optimum conditions were detd. for preparative electrooxygenation of hydrocarbons and a mechanistic hypothesis was proposed where binuclear iron complexes were thought to intervene.
IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidn. catalysts, for electrochem. oxidn. of satd. hydrocarbons by Gif-Orsay system)

L58 ANSWER 30 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:631449 HCAPLUS
DOCUMENT NUMBER: 111:231449
TITLE: Hydrocarbon oxidations catalyzed by azide- or nitride-activated metal coordination complexes
INVENTOR(S): Ellis, Paul E.; Lyons, James E.; Myers, Harry K.
PATENT ASSIGNEE(S): Sun Refining and Marketing Co., USA
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 11

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 274909	A2	19880720	EP 1987-311480	19871229
EP 274909	A3	19900207		
EP 274909	B1	19940810		
R: BE, DE, FR, GB, IT, NL				
US 4895682	A	19900123	US 1987-246	19870102
US 4895680	A	19900123	US 1987-247	19870102
CA 1302433	A1	19920602	CA 1987-553416	19871203
CA 1336188	A1	19950704	CA 1987-553420	19871203
NO 8705496	A	19880704	NO 1987-5496	19871230
NO 169710	B	19920421		
NO 169710	C	19920729		
SU 1833358	A3	19930807	SU 1987-4203962	19871231
JP 01180840	A2	19890718	JP 1988-46	19880104
JP 2517340	B2	19960724		
US 5663328	A	19970902	US 1996-672202	19960627

PRIORITY APPLN. INFO.:

US 1987-246	19870102
US 1987-247	19870102
US 1987-66666	19870626
US 1989-425089	19891023
US 1990-568116	19900816
US 1994-303106	19940907

OTHER SOURCE(S): CASREACT 111:231449

AB The title process is used in the prepn. of alcs., ketones, acids, esters, or mixts. thereof. For example, oxidn. of 7 g isobutane in C6H6 at 80.degree. and 75 psig O2 for 6 h in the presence of 0.025 mmol Co(L)N3 [L = 1,3-bis(2-pyridylimino)isoindoline] gave a turn over no. of 196 which was quite superior to Co(L)(OAc) or Co(acac)2 with added NaN3. Products were Me3COH and Me2CO.

IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for oxidn. of hydrocarbons)

L58 ANSWER 31 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:630002 HCAPLUS
DOCUMENT NUMBER: 109:230002
TITLE: Monooxygenase-like oxidation of hydrocarbons by hydrogen peroxide catalyzed by manganese porphyrins and imidazole: selection of the best catalytic system and nature of the active oxygen species
AUTHOR(S): Battioni, P.; Renaud, J. P.; Bartoli, J. F.; Reina-Artiles, M.; Fort, M.; Mansuy, Daniel
CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., CNRS, Paris, 75270, Fr.
SOURCE: Journal of the American Chemical Society (1988), 110(25), 8462-70
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:230002

AB Fe and Mn porphyrins alone are almost unable to catalyze cyclooctene epoxidn. or cyclooctane hydroxylation by H2O2. In the presence of imidazole, Mn(III) porphyrins, and particularly Mn(TDCPP)Cl, are much better catalysts than Fe porphyrins for oxygen-atom transfer from H2O2 to hydrocarbons. From a study of various Mn porphyrin catalysts and nitrogen base cocatalysts, the most efficient system that has been selected involves Mn(TDCPP)Cl in the presence of 10-20 equiv of imidazole. This system leads to high yields of alkene epoxidn. (90-100% in less than 1 h at room temp.). Epoxidn. of 1,2-dialkylethylenes is stereospecific and corresponds to a syn addn. of an oxygen atom to the double bond. This

system also leads to the oxidn. by H2O2 of various alkanes such as cyclohexane, cyclooctane, adamantane, ethylbenzene or tetralin, with formation of the corresponding alcs. and ketones in yields between 40 and 80%. The Mn(TDCPP)Cl-imidazole-PhIO and Mn(TDCPP)Cl-imidazole-H2O2 systems exhibit the following: (i) identical stereospecificities for the epoxidn. of stilbene and hex-2-ene, (ii) identical regioselectivities for the epoxidn. of isoprene and limonene as well as for the hydroxylation of n-heptane, and (iii) almost identical chemoselectivities for the oxidn. of cyclohexene and of mixts. of cyclooctane. This indicates that very similar, if not identical, high-valent Mn-oxo-intermediates are the active oxygenating species in both systems. Thus, thanks to the presence of imidazole, it is possible to perform efficient biomimetic monooxygenations of hydrocarbons by using the Mn(TDCPP)Cl catalyst and H2O2 instead of PhIO as the oxygen-atom donor.

IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalytic activity of, in oxidn. of hydrocarbons)

L58 ANSWER 32 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:11084 HCAPLUS
DOCUMENT NUMBER: 104:11084
TITLE: Steric and electronic control of iron porphyrin catalyzed hydrocarbon oxidations
AUTHOR(S): Nappa, Mario J.; Tolman, Chadwick A.
CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Inc., Wilmington, DE, 19898, USA
SOURCE: Inorganic Chemistry (1985), 24(26), 4711-19
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The yields and product distributions in the oxidn. of hydrocarbons (cyclohexane, pentane, octane, methylcyclohexane, tert-butylcyclohexane, and ethylbenzene), with substituted Fe tetraphenylporphyrins and iodosobenzene, are affected by the nature and location of Ph ring substituents. These substrates were used to measure the activity, regioselectivity, substrate selectivity, and stereoselectivity of these substituted Fe porphyrin catalysts. Higher yields are obsd. with Fe porphyrins having bulky substituents near the Fe center. Kinetics measurements and concn. studies show that these substituents improve lifetimes by hindering catalyst bimol. self-destruction. Higher yields are also obsd. with electron-withdrawing substituents. A new Fe fluoro-pocket porphyrin shows high activity due to this electronic effect. Substrate and regioselectivity are also influenced by steric and electronic effects of the Fe porphyrin Ph ring substituents. Bulky porphyrins also affect the stereoselectivity at the 2-, 3- and 4-positions in tert-butylcyclohexane oxidn. A mechanism supported by kinetic modeling studies is proposed for the oxidn. reactions.

IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for oxidn. of hydrocarbons)

L58 ANSWER 33 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:504796 HCAPLUS
DOCUMENT NUMBER: 99:104796
TITLE: Conversion of an alkane to a mixture of an alcohol and a ketone
INVENTOR(S): Middleton, Anthony Robert; Smith, David John Harry
PATENT ASSIGNEE(S): British Petroleum Co. PLC, UK
SOURCE: Eur. Pat. Appl., 14 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 79705	A1	19830525	EP 1982-305724	19821028
R: BE, DE, FR, GB, IT, NL				
US 4459427	A	19840710	US 1982-436785	19821026
AU 8289819	A1	19830505	AU 1982-89819	19821027
CA 1215388	A1	19861216	CA 1982-414477	19821029
JP 58085827	A2	19830523	JP 1982-192351	19821101
PRIORITY APPLN. INFO.:			GB 1981-32870	19811031
			GB 1981-32871	19811031

AB Alkanes were oxidized by hydrocarbyl hydroperoxides using a Fe or Mn square planar complex that had heterocyclic N donor ligands and weakly coordinating, non-coordinating, or no axial ligands, to give alcs. and ketones. Thus cyclohexane was treated with Me3COOH and Fe(tetraphenylporphyrin) to give 18% cyclohexanol and 35% cyclohexanone.

IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(oxidn. catalyst, for hydrocarbons with hydroperoxides)

L58 ANSWER 34 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:521435 HCAPLUS
DOCUMENT NUMBER: 99:121435
TITLE: Catalytic replacement of unactivated alkane carbon-hydrogen bonds with carbon-X bonds (X = nitrogen, oxygen, chlorine, bromine, or iodine). Coupling of intermolecular hydrocarbon activation by MnIIITPPX complexes with phase-transfer catalysis
AUTHOR(S): Hill, Craig L.; Smegal, John A.; Henly, Timothy J.
CORPORATE SOURCE: Dep. Chem., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Journal of Organic Chemistry (1983), 48(19), 3277-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:121435

AB The title reaction system is composed of 2 liq. phases and the oxidant PhIO. The alkane substrate, the MnIII TPPX catalyst, and the org. solvent (CH2Cl2, PhCl, or other arom. hydrocarbon) constitute 1 phase, a satd. aq. soln. of the Na salt of the anion to be incorporated into the alkane constitutes the 2nd phase, and the sparingly sol. PhIO constitutes a 3rd phase. When the 2 liq. phases and PhIO are stirred under an inert atm., both RX and ROH products are produced catalytically based on MnTPP, and in reasonable yield based on PhIO. The MnTPP moiety functions as a catalyst for C-H bond cleavage and for phase transfer of X- from the aq. phase to the org. phase, where the functionalization chem. takes place. ClO- can be used in place of, but is less effective than, PhIO, whereas H2O2, IO4- and S2O82- are ineffective. Product distributions obtained from the oxidn. of cyclohexane, Me3CH, Me2CHCHMe2 and PhCMe3 are most consistent with a product-detg. step involving transfer of X from Mn to a free alkyl-radical intermediate.

IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for phase-transfer functionalization of alkanes in presence of iodosobenzene)

L58 ANSWER 35 OF 47 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1982:455050 HCAPLUS
DOCUMENT NUMBER: 97:55050
TITLE: Biomimetic **oxidation** of **organic** sulfides with meso-tetraphenylporphyriniron chloride/imidazole/hydrogen peroxide
AUTHOR(S): Oae, Shigeru; Watanabe, Yoshihito; Fujimori, Ken

CORPORATE SOURCE: Dep. Chem., Univ. Tsukuba, Ibaraki, 305, Japan
SOURCE: Tetrahedron Letters (1982), 23(11), 1189-92
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enzyme model system meso-tetraphenylporphyriniron(III) chloride-imidazole catalyzed the S-oxygenation and oxidative S-dealkylation of org. sulfides with H2O2. The effect of para substitution on the rate of sulfoxidn. of PhSMe was studied. Electron-releasing groups accelerated S-oxidn., and there was good correlation between kinetics and 1-electron oxidn. potentials of the corresponding sulfides and with Brown-Okamoto .sigma.+ substituent consts.; the reaction const., .rho.+, was -0.26. Oxidn. of the benzothiophene I with this system gave the corresponding trans-sulfoxide stereoselectivity. Thus, this biomimetic oxidn. showed reasonable similarity to the enzymic oxidn. with cytochrome P-450.
IT **16456-81-8**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, imidazole and, for **oxidn.** of **org.** sulfides)

L58 ANSWER 36 OF 47 USPATFULL
ACCESSION NUMBER: 2003:47732 USPATFULL
TITLE: Main-group metal based asymmetric catalysts and applications thereof
INVENTOR(S): Jacobsen, Eric N., Boston, MA, United States
Sigman, Matthew S., Somerville, MA, United States
PATENT ASSIGNEE(S): President and Fellows of Harvard College, Cambridge, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6521561	B1	20030218
APPLICATION INFO.:	US 1998-71842		19980501 (9)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Wood, Elizabeth D.
LEGAL REPRESENTATIVE: Gordon, Dana M., Foley Hoag LLP
NUMBER OF CLAIMS: 35
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)
LINE COUNT: 2398
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention relates to a method and catalysts for the stereoselective addition of a nucleophile to a reactive .pi.-bond of a substrate. The chiral, non-racemic catalysts of the present invention constitute the first examples of catalysts for nucleophilic additions that comprise a main-group metal and a tri- or tetra-dentate ligand.

L58 ANSWER 37 OF 47 USPATFULL
ACCESSION NUMBER: 2002:119566 USPATFULL
TITLE: Stabilized proteins
INVENTOR(S): Marshall, Christopher P., Brooklyn, NY, UNITED STATES
Hoffman, Alexander, Los Angeles, CA, UNITED STATES
Errico, Joseph P., Far Hills, CA, UNITED STATES
Marshall, Paul B., Munich, GERMANY, FEDERAL REPUBLIC OF

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002061549	A1	20020523
APPLICATION INFO.:	US 2001-837235	A1	20010418 (9)

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. WO 2000-US28595, filed on 16 Oct 2000, UNKNOWN

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-159763P	19991015 (60)

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: PENNIE AND EDMONDS, 1155 AVENUE OF THE AMERICAS, NEW YORK, NY, 100362711
NUMBER OF CLAIMS: 20
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 26 Drawing Page(s)
LINE COUNT: 5385
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention described herein comprises methods for stabilizing polypeptides and polypeptide complexes, and the polypeptides and polypeptide complexes stabilized using the methods. To achieve stabilization, a cross-link reaction is controlled such that polypeptides and polypeptide complexes maintain their original functionality. In one embodiment, the invention provides a method for the identification of amino acid residues which, when cross-linked, are least disruptive to the structure and function of the polypeptide or polypeptide complex. In another embodiment, the invention provides a method for mutagenesis of identified residues to further control the cross-link reaction. Polypeptides and polypeptide complexes so stabilized can be utilized under a wide variety of physiological and non-physiological conditions. Further, the cross-link methodology disclosed herein may preclude the need for addition of exogenous structures to engineered proteins and complexes, such as peptide linkers that could be immunogenic and/or significantly decrease efficacy. In another embodiment, the invention provides a method for statistical analysis of databases of structural and/or sequence information available for polypeptides and polypeptide complexes to be stabilized. The statistical analysis identifies suitable residue pairs which are least likely to be disruptive of structure and function when cross-linked. Further, in a polypeptide chain or chains to be cross-linked, potentially undesirable reactive side-chains may be masked and protected, or altered using site-directed mutagenesis, e.g., to introduce a maximally conservative point mutation that will not support the cross-link reaction. The cross-link reaction conditions may also be adjusted to prevent undesired cross-links or other undesired side-effects. At residues identified as desirable positions for cross-linking, reactive side-chains may be introduced by site-directed mutagenesis, and the cross-link reaction is carried out using the conditions identified above.

L58 ANSWER 38 OF 47 USPATFULL
ACCESSION NUMBER: 2002:137161 USPATFULL
TITLE: Non-genotoxic metalloporphyrins as synthetic catalytic scavengers of reactive oxygen species
INVENTOR(S): Meunier, Bernard, Castanet, FRANCE
Cosledan, Frederic, Escalquens, FRANCE
PATENT ASSIGNEE(S): Eukarion, Inc., Bedford, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6403788	B1	20020611
APPLICATION INFO.:	US 2000-613891		20000711 (9)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Raymond, Richard L.
ASSISTANT EXAMINER: Habte, Kahsay
LEGAL REPRESENTATIVE: Hamilton, Brook, Smith & Reynolds, P.C.

NUMBER OF CLAIMS: 39
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 2 Drawing Figure(s); 2 Drawing Page(s)
LINE COUNT: 1759
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB This invention relates to compounds which are non-genotoxic metalloporphyrins. These compounds are synthetic catalytic scavengers of reactive oxygen chemical species. The invention also relates to pharmaceutical compositions comprising these compounds and to methods of use of these compounds for preventing or arresting free radical associated diseases or conditions.

L58 ANSWER 39 OF 47 USPATFULL
ACCESSION NUMBER: 2002:88274 USPATFULL
TITLE: Biomimetic reagent system and its use
INVENTOR(S): Bather, Wolfgang, Lubeck, GERMANY, FEDERAL REPUBLIC OF
Duchstein, Hans-Jurgen, Pinneberg, GERMANY, FEDERAL REPUBLIC OF
Hoffmann, Susanne, Buchholz, GERMANY, FEDERAL REPUBLIC OF
PATENT ASSIGNEE(S): Drager Sicherheitstechnik GmbH, GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6376254	B1	20020423	
APPLICATION INFO.:	US 1999-394969		19990910	(9)

	NUMBER	DATE
PRIORITY INFORMATION:	DE 1999-19912380	19990319

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Snay, Jeffrey
LEGAL REPRESENTATIVE: McGlew and Tuttle, P.C.
NUMBER OF CLAIMS: 30
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 1 Drawing Figure(s); 1 Drawing Page(s)
LINE COUNT: 480
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A biomimetic reagent system is provided containing an oxygen donor and a catalyst based on porphyrin, which are applied to a carrier. A device that contains the system is also provided for determining components of gas or vapor samples, especially aromatics, such as benzene. A process for hydroxylating aromatics, such as benzene, using the biomimetic reagent system is also provided.

L58 ANSWER 40 OF 47 USPATFULL
ACCESSION NUMBER: 2001:86409 USPATFULL
TITLE: Methanol tolerant catalyst material
INVENTOR(S): Chu, Dervn, Havertown, PA, United States
Jiang, Rongzbong, Gaithersburg, MD, United States
PATENT ASSIGNEE(S): The United States of America as represented by the Secretary of the Army, Washington, DC, United States (U.S. government)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6245707	B1	20010612	
APPLICATION INFO.:	US 1999-429702		19991028	(9)

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Wood, Elizabeth D.

LEGAL REPRESENTATIVE: Clohan, Jr., Paul S.
NUMBER OF CLAIMS: 16
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 9 Drawing Figure(s); 9 Drawing Page(s)
LINE COUNT: 639
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Methanol tolerant catalyst materials and a method of making the same are provided. These novel catalyst materials are obtained by mixing together and heat-treating at least two different transition-metal-containing nitrogen chelates. In preferred embodiments, the nitrogen chelates comprise metalloporphyrins such as transition-metal-containing tetraphenylporphins. Preferred transition metals are iron, cobalt, nickel, copper, manganese, ruthenium, vanadium, and zinc, but could be any transition metal other than platinum or palladium. These materials offer improved catalytic oxygen reduction in the presence of methanol, as may occur at a fuel cell cathode after methanol crossover.

L58 ANSWER 41 OF 47 USPATFULL
ACCESSION NUMBER: 2000:128484 USPATFULL
TITLE: Octafluoro-meso-tetraarylporphyrins and methods for making these compounds
INVENTOR(S): DiMagno, Stephen G., Lincoln, NE, United States
PATENT ASSIGNEE(S): University of Nebraska-Lincoln, Lincoln, NE, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6124452		20000926	
APPLICATION INFO.:	US 1997-994891		19971219	(8)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Shah, Mukund J.
ASSISTANT EXAMINER: Sripada, Pavanaram K
LEGAL REPRESENTATIVE: Shook, Hardy & Bacon LLP
NUMBER OF CLAIMS: 34
EXEMPLARY CLAIM: 1
LINE COUNT: 785
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The novel compounds of the present invention are .beta.-octafluoro-meso-tetraarylporphyrins of formula (I) and their metallic complexes of formula (II): ##STR1## .beta.-octafluoro-meso-tetraaryl porphyrins are synthesized by reacting 3,4-difluoropyrrole with an aromatic aldehyde in the presence of boron trifluoride etherate, followed by **oxidation**. The difluoropyrrole used in this reaction is produced by reacting 3,3,4,4-tetrafluoropyrroline or its corresponding salt, 3,3,4,4-tetrafluoropyrrolidinium salt, with a base such as potassium tert-butoxide. The metalloporphyrins of the present invention are synthesized by deprontonating .beta.-octafluoro-meso-tetraarylporphyrin ligands and treating said ligands with metal ions.

L58 ANSWER 42 OF 47 USPATFULL
ACCESSION NUMBER: 2000:106075 USPATFULL
TITLE: Catalyst that **oxidizes** steroids and other substrates with catalytic turnover
INVENTOR(S): Breslow, Ronald, Englewood, NJ, United States
Yang, Jerry, New York, NY, United States
Gabriele, Bartolo, New York, NY, United States
PATENT ASSIGNEE(S): The Trustees of Columbia University in the City of New York, New York, NY, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6103892		20000815

APPLICATION INFO.: US 1998-57417 19980408 (9)
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Kunz, Gary L.
LEGAL REPRESENTATIVE: White, John P.Cooper & Dunham LLP
NUMBER OF CLAIMS: 23
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 11 Drawing Figure(s); 5 Drawing Page(s)
LINE COUNT: 678
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides a metalloporphyrin catalyst represented by the structure: ##STR1##

L58 ANSWER 43 OF 47 USPATFULL
ACCESSION NUMBER: 2000:21519 USPATFULL
TITLE: Metalloporphyrin **oxidation** catalyst covalently coupled to an inorganic surface and method making same
INVENTOR(S): Ying, Jackie Y., Winchester, MA, United States
Zhang, Lei, Cambridge, MA, United States
Sun, Tao, Midland, MI, United States
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, Cambridge, MA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6028025		20000222
APPLICATION INFO.:	US 1996-734170		19961021 (8)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Straub, Gary P.
ASSISTANT EXAMINER: Vanoy, Timothy C
LEGAL REPRESENTATIVE: Wolf, Greenfield & Sacks, P.C.
NUMBER OF CLAIMS: 25
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 23 Drawing Figure(s); 20 Drawing Page(s)
LINE COUNT: 1111
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A system is provided including an article having a surface and a catalytic metal atom, capable of **oxidation**, covalently immobilized at the surface via a plurality of covalent bonds, but being free of direct covalent bonding to the surface. In particular, the invention relates to inorganic surfaces including silica, alumina, niobium **oxide**, or tantalum **oxide**, or a combination thereof and catalytic metal atoms including Fe, Mn, Cr, Ni, Co, Ru, and Os. The catalytic metal atom, covalently immobilized at the surface via a plurality of covalent bonds, can be immobilized via bonding through at least one atom that is bonded directly to the surface. The article preferably is an inorganic, mesoporous structure, in the pores of which are covalently bonded a plurality of metalloporphyrins. In particular, the catalytic metal atom, such as iron, manganese, chromium, nickel, cobalt, rhenium, and osmium are covalently bonded to a porphyrin structure which is bonded to an alumina or silica surface via bonds between the amine groups of the porphyrin structure of the alumina or silica surface. The invention also discloses supporting the catalytic metal atom bonded to the porphyrin structure via amine groups in the porphyrin and dopant atoms of the alumina or silica surface. Dopant atoms can include niobium and tantalum atoms.

L58 ANSWER 44 OF 47 USPATFULL
ACCESSION NUMBER: 1999:163881 USPATFULL
TITLE: Catalytic oxygenation of hydrocarbons by metalloporphyrin and metallosalen complexes

INVENTOR(S): Groves, John T., Princeton, NJ, United States
Carofiglio, Tommaso, Padua, Italy
Bonchio, Marcella, Padua, Italy
Sauve, Anthony, Princeton, NJ, United States
PATENT ASSIGNEE(S): The Trustees of Princeton University, Princeton, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6002026		19991214
APPLICATION INFO.:	US 1996-760849		19961205 (8)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1996-686663, filed on 26 Jul 1996, now abandoned
DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Kight, John
ASSISTANT EXAMINER: Desai, Rita
LEGAL REPRESENTATIVE: Hoffmann & Baron, LLP
NUMBER OF CLAIMS: 10
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 5 Drawing Figure(s); 5 Drawing Page(s)
LINE COUNT: 964
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to novel **oxidative** processes for substrates such as olefins, alkanes, aromatics and alcohols using metallic porphyrin or salen catalytic complexes which have been specifically designed to maximize catalytic activity, thereby enhancing efficiency, selectively and speed of **oxidation** of these substrates. The choice of the substituents in the metallic complexes may be varied, but must be chosen to prevent specific ligand set arrangements known to be stable and therefore less catalytically efficient. Coordination complexes, particularly porphyrins and salens having nitrosyl axial ligands and electron-withdrawing peripheral substituents are preferred. Ruthenium coordination metals are the preferred metal center, with the highly reactive catalytic species found to be Ru.sup.III.

L58 ANSWER 45 OF 47 USPATFULL
ACCESSION NUMBER: 1998:88995 USPATFULL
TITLE: Process for the preparation of a mixture of guaiacol and p-methoxy phenol
INVENTOR(S): Moghe, Pramod Prabhakar, Pune, India
Ratnasamy, Paul, Pune, India
Raja, Robert, Madras, India
Pol, Ashwini Vinayak, Pune, India
Kotasthane, Madhav Gopal, Pune, India
Bahirat, Prakash Kondiba, Pune, India
PATENT ASSIGNEE(S): Council of Scientific & Industrial Research, New Dehli, India (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5786519		19980728
APPLICATION INFO.:	US 1996-602600		19960216 (8)

DOCUMENT TYPE: Utility
FILE SEGMENT: Granted
PRIMARY EXAMINER: Robinson, Allen J.
ASSISTANT EXAMINER: Badio, Barbara
LEGAL REPRESENTATIVE: Greenlee, Winner and Sullivan, P.C.
NUMBER OF CLAIMS: 14
EXEMPLARY CLAIM: 1
LINE COUNT: 434
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB An improved process is provided for the preparation of a mixture of guaiacol and p-methoxy phenol which comprises reacting anisole with hydrogen peroxide in the presence of a solid catalyst containing an organotransition metal complex wherein some or all of the hydrogen atoms of the said organotransition metal complex have been substituted by one or more electron withdrawing groups, and isolating the mixture of guaiacol and p-methoxy phenol formed.

L58 ANSWER 46 OF 47 USPATFULL

ACCESSION NUMBER:	97:18278 USPATFULL
TITLE:	Porphyrins and metal complexes thereof having haloalkyl side chains
INVENTOR(S):	Wijesekera, Tilak, Glen Mills, PA, United States Lyons, James E., Wallingford, PA, United States Ellis, Jr., Paul E., Downingtown, PA, United States Bhinde, Manoj V., Boothwyn, PA, United States
PATENT ASSIGNEE(S):	Sun Company, Inc. (R&M), Philadelphia, PA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5608054		19970304
APPLICATION INFO.:	US 1995-405684		19950317 (8)

RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1993-174732, filed on 29 Dec 1993 And a continuation-in-part of Ser. No. US 1993-175057, filed on 29 Dec 1993
DOCUMENT TYPE:	Utility
FILE SEGMENT:	Granted
PRIMARY EXAMINER:	Datlow, Philip I.
LEGAL REPRESENTATIVE:	Dickinson, Q. Todd, Falk, Stephen T.
NUMBER OF CLAIMS:	8
EXEMPLARY CLAIM:	1,8
NUMBER OF DRAWINGS:	7 Drawing Figure(s); 7 Drawing Page(s)
LINE COUNT:	384

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Transition metal complexes of meso-haloalkylporphyrins, wherein the haloalkyl groups contain 2 to 8 carbon atoms have been found to be highly effective catalysts for **oxidation** of alkanes and for the decomposition of hydroperoxides.

L58 ANSWER 47 OF 47 USPATFULL

ACCESSION NUMBER:	96:101672 USPATFULL
TITLE:	Porphyrins
INVENTOR(S):	Wijesekera, Tilak, Glen Mills, PA, United States Lyons, James E., Wallingford, PA, United States Ellis, Jr., Paul E., Downingtown, PA, United States
PATENT ASSIGNEE(S):	Sun Company, Inc. (R&M), Philadelphia, PA, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5571908		19961105
APPLICATION INFO.:	US 1993-174732		19931229 (8)

RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1990-568116, filed on 16 Aug 1990 which is a continuation-in-part of Ser. No. US 1989-425089, filed on 23 Oct 1989, now abandoned which is a continuation-in-part of Ser. No. US 1987-66666, filed on 26 Jun 1987, now patented, Pat. No. US 4900871 which is a continuation-in-part of Ser. No. US 1987-246, filed on 2 Jan 1987, now patented, Pat. No. US 4895682
DOCUMENT TYPE:	Utility
FILE SEGMENT:	Granted

PRIMARY EXAMINER: Datlow, Philip I.
LEGAL REPRESENTATIVE: Dickinson, Q. Todd, Falk, Stephen T.
NUMBER OF CLAIMS: 13
EXEMPLARY CLAIM: 1
LINE COUNT: 598
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention comprises new compositions of matter, which are iron, manganese, cobalt or ruthenium complexes of porphyrins having hydrogen, haloalkyl or haloaryl groups in meso positions, two of the opposed meso atoms or groups being hydrogen or haloaryl, and two of the opposed meso atoms or groups being hydrogen or haloalkyl, but not all four of the meso atoms or groups being hydrogen. The invention also comprises new compositions of matter in which all four of the meso positions are substituted with haloalkyl groups and the beta positions are substituted with halogen atoms. A new method of synthesizing porphyrinogens is also provided.

The novel compositions and others made according to the process of the invention are useful as hydrocarbon conversion catalysts; for example, for the **oxidation** of alkanes and the decomposition of hydroperoxides.

```
=> fil casreact; d stat que l61
FILE 'CASREACT' ENTERED AT 11:49:48 ON 15 MAY 2003
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FILE CONTENT:1907 - 11 May 2003 VOL 138 ISS 19

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file
and provided by InfoChem and some records are produced using some INPI
data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

Crossover limits have been increased.  See HELP RNCROSSOVER for details.

Structure search limits have been raised.  See HELP SLIMIT for the new,
higher limits.
```
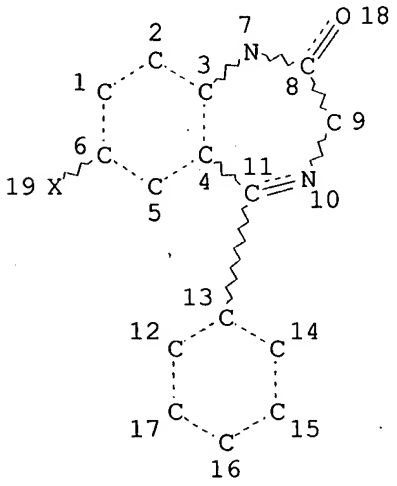

L59 reactant or reagent STR

RRT



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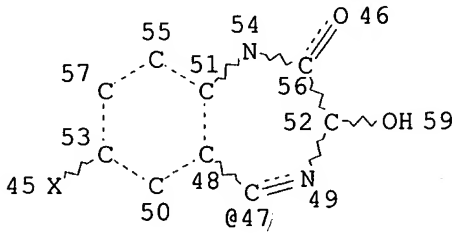
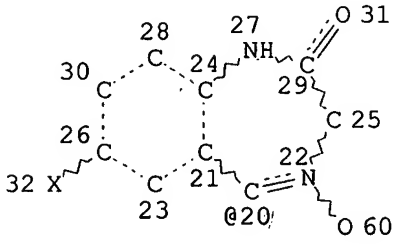


X = any halogen

Page 1-A

PRO



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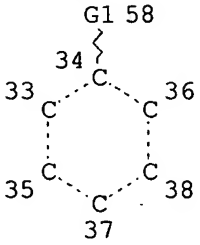

Page 2-A
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 54

STEREO ATTRIBUTES: NONE
L61 24 SEA FILE=CASREACT SSS FUL L59 (84 REACTIONS)

100.0% DONE 338 VERIFIED 84 HIT RXNS 24 DOCS
SEARCH TIME: 00.00.01

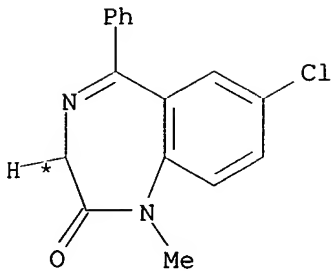
=> d ibib abs fhit l61 1-24; fil hom

L61 ANSWER 1 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 134:178573 CASREACT
TITLE: Process for the metalloporphyrin catalyzed oxidation of organic compounds
INVENTOR(S): Bernardelli, Patrick
PATENT ASSIGNEE(S): Warner Lambert Company, USA
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001010797	A1	20010215	WO 2000-EP7726	20000809
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000013018	A	20020416	BR 2000-13018	20000809
EP 1208069	A1	20020529	EP 2000-960420	20000809
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506419	T2	20030218	JP 2001-515270	20000809
PRIORITY APPLN. INFO.:			US 1999-148079P	19990810
			US 1999-150101P	19990820
			WO 2000-EP7726	20000809

AB An org. compd. (e.g., Diazepam) is oxidized using a catalytic amt. of metalloporphyrin (tetrakis(pentafluorophenylporphyrin)manganese (III) chloride) and an oxidizing agent (iodosyl benzene, hydrogen peroxide) in an inert, aprotic, polyhalogenated solvent (benzotrifluoride). Oxidn. of diazepam is conducted to mimic oxidn. (metab.) in biol. systems. The products of the oxidn. of diazepam are sepd. and quantitated. A polar, non-nucleophilic co-solvent may be used (hexafluoroisopropanol, trifluoroethanol) in the range of 1-30%. The reaction may be biphasic and use a phase-transfer catalyst (dodecyl trimethylammonium bromide). Use of an inert aprotic solvent shows improved oxidn. yields when compared to prior art (e.g., CH3CN-CH2Cl2-water mixts.).

RX(1) OF 8 4 **A** ===> B + **C** + D + E



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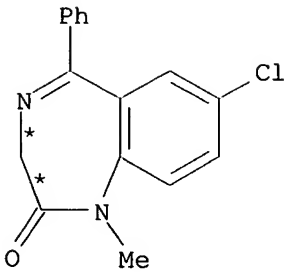

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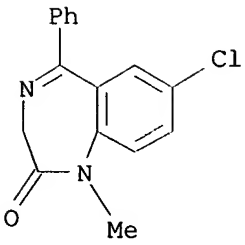

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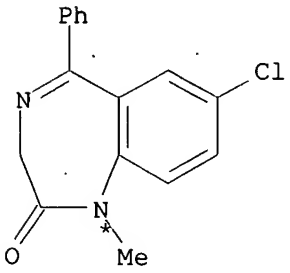

A

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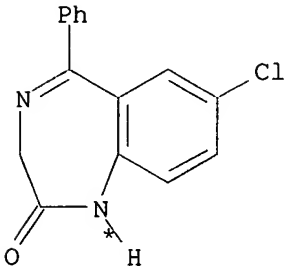
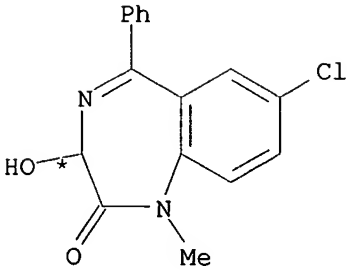


B
YIELD 4%



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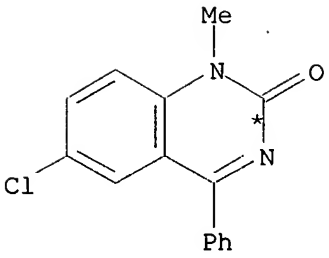
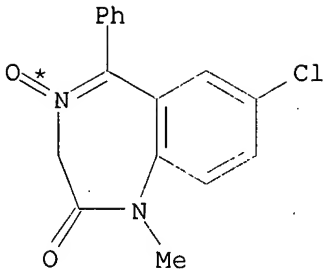
YIELD 7%



D
YIELD 1%



E
YIELD 5%

RX(1) RCT A **439-14-5**

STAGE(1)
SOL 98-08-8 Benzene, (trifluoromethyl)-

STAGE(2)
CAT 79968-43-7 Manganese, chloro[5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-porphinato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-12)-, 920-66-1 (F3C)2CHOH
SOL 98-08-8 Benzene, (trifluoromethyl)-

STAGE(3)
RGT F 7722-84-1 H2O2
SOL 7732-18-5 Water

STAGE(4)
CAT 288-32-4 1H-Imidazole
SOL 7732-18-5 Water

STAGE(5)
CAT 631-61-8 NH4OAc
SOL 7732-18-5 Water

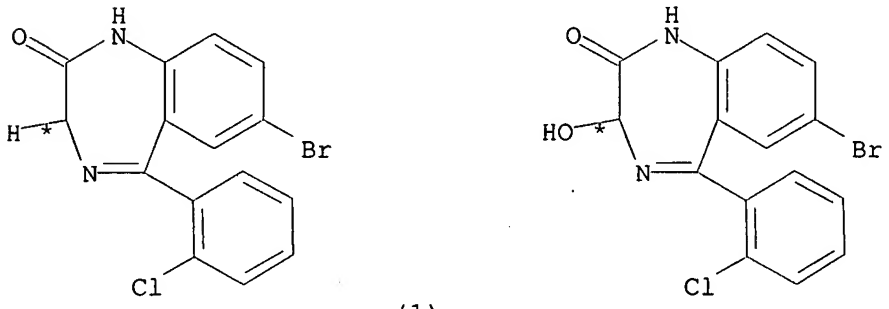
PRO B 1088-11-5, C **846-50-4**, D 20927-53-1, E 2888-64-4
NTE 1 EQUIV. PEROXIDE, PHASE-TRANSFER CATALYSIS

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 2 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 129:290114 CASREACT
TITLE: Oxidation of nitrogen-containing heterocycles using biocatalysts
AUTHOR(S): Davidenko, T. I.
CORPORATE SOURCE: A. V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, 270080, Ukraine
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1998), 47(8), 1565-1570
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method for stereospecific hydroxylation of 1,2-dihydro-3H-1,4-benzodiazepin-2-ones using free and immobilized cells of Actinomycetes as

biocatalysts was developed. The hydroxylation under the action of yeast results in the formation of racemates. Actinomyces do not hydroxylate quinazolinones, quinoxalinones, and tetrahydro-1,5-benzodiazepin-2-ones; derivs. of 1,2,3,4-tetrahydro-1,5-benzodiazocin-2-ones are transformed into 2-[N-(3-acetylaminopropionyl)amino]benzophenones.

RX(1) OF 15 **A** ===> **B**



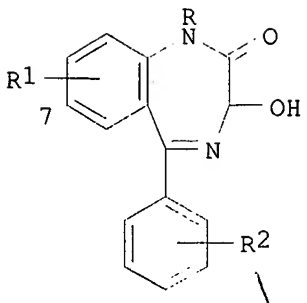
RX(1) RCT A **51753-57-2**
PRO B **214194-35-1**
SOL 67-68-5 DMSO
NTE BIOTRANSFORMATION, ENZYMIC HYDROXYLATION, ACTINOMYCES ROSEOCHROMOGENES
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 3 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 122:10073 CASREACT
TITLE: Method for production of 1,4-benzodiazepine derivatives
INVENTOR(S): Krawczynska, Bogumila; Morawski, Bogdan; Kalis, Jadwiga; Chojnacka, Romualda
PATENT ASSIGNEE(S): Tarchominskie Zaklady Farmaceutyczne "Polfa", Pol.
SOURCE: Pol., 4 pp.
CODEN: POXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Polish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 158635	B1	19920930	PL 1988-272101	19880427

PRIORITY APPLN. INFO.: PL 1988-272101 19880427
OTHER SOURCE(S): MARPAT 122:10073
GI

uses ~~includes~~ solvent excluded by prov 130



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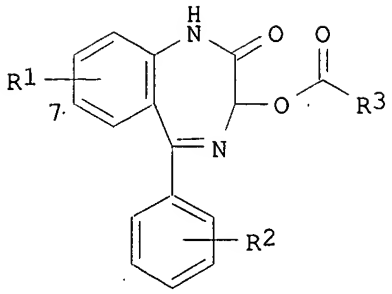
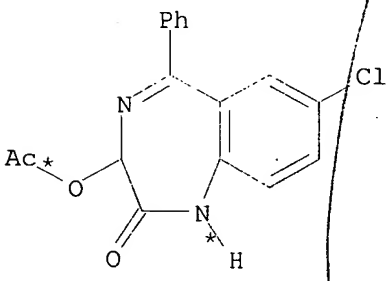


II

AB Benzodiazepine derivs. I [R = (un)substituted C1-4 alkyl; R1, R2 = H, halo, nitro] are prepd. by simultaneous hetero-phase hydrolysis and alkylation of benzodiazepine esters II [R3 = C1-3 alkyl] in a system comprising a water-insol. org. solvent and an aq. soln. of an alkali metal hydroxide, in the presence of a quaternary ammonium salt (phase-transfer catalyst), and under the action of an alkylating agent RX (X = halo). For example, a suspension of II [R1 = 7-Cl, R2 = H, R3 = Me] in a mixt. of CH2Cl2, aq. 40% NaOH, and Bu4N+ Cl-, was stirred 1 h at 20-25.degree., dild. with H2O, treated dropwise with MeI, and stirred 3 h at 25-30.degree., to give I [R = Me, R1 = 7-Cl, R2 = H] in 85% yield with m.p. 159-160.degree.. A similar prepn. using KOH and PhCH2N+Et3 Cl- in ClCH2CH2Cl gave 89% yield. Also prepd. were I [R = Me, R1 = 7-Cl, R2 = o-Cl] in 87% yield, and I.HCl [R = CH2CH2NEt2, R1 = 7-Cl, R2 = o-F] in 79% yield.

RX(1) OF 4 **A** + B ===> **C**



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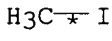

B

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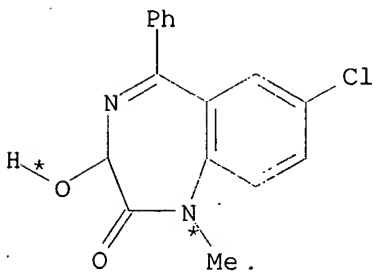


C
YIELD 85%

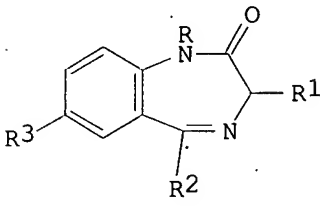
RX(1) RCT A **1824-74-4**

STAGE(1)
RGT D 1310-73-2 NaOH
CAT 1643-19-2 Bu4N.Br
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

solvent excluded by proviso

STAGE(2)
RCT B 74-88-4
PRO C **846-50-4**

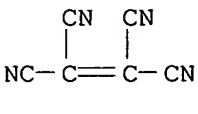
L61 ANSWER 4 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 114:246735 CASREACT
TITLE: Characteristics of charge transfer of 1,4-benzodiazepin-2-ones
AUTHOR(S): Ying, Baining; Ouyang, Jiexiang; Xu, Xiangong
CORPORATE SOURCE: Dep. Chem., Zhongshan Univ., Guangzhou, 510275, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1990), 11(11), 1254-8
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

AB The interaction of 1,4-benzodiazepin-2-ones I (R = H, Me; R1 = H, OH, BzO, AcO; R2 = Ph, 2-pyridyl, 2-ClC6H4; R3 = H, Br, Cl, iodo, cyano, NO2, NH2, NHAc) with tetracyanoethylene or potassium p-methylphenoxide can form charge transfer complexes. By a spectrophotometric method the electron affinity and the ionization potential of the title compds. are calcd. with the energy of electron transfer. The thermodn. consts. of the complexes are detd. as well. 1,4-Benzodiazepin-2-ones can act not only as charge acceptor but also as charge donor.

RX(17) OF 20 A + **R** ===> **S**



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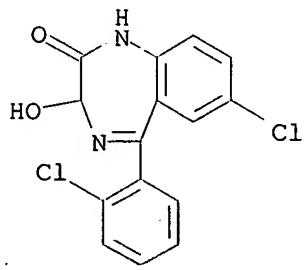
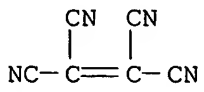


R

(17)



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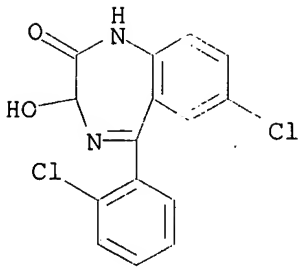
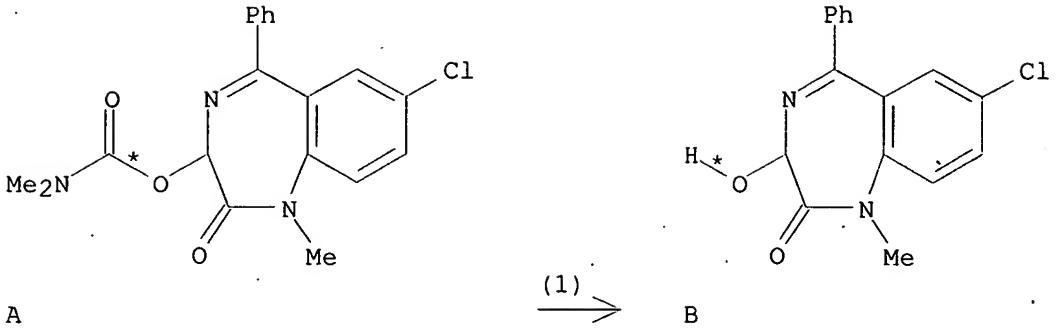


S: CM 2

RX(17) RCT A 670-54-2, R **846-49-1**
PRO S **134070-75-0**

L61 ANSWER 5 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 114:220623 CASREACT
TITLE: Voltammetric studies on the interactions between camazepam metabolic series and human serum albumin. Determination of oxazepam using adsorptive stripping voltammetry
AUTHOR(S): Zapardiel, A.; Perez Lopez, J. A.; Bermejo, E.; Hernandez, L.; Chicharro, M.
CORPORATE SOURCE: Dep. Anal. Chem., Auton. Univ., Madrid, 28049, Spain
SOURCE: Analytica Chimica Acta (1991), 244(1), 49-57
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The behavior of oxazepam in adsorptive stripping voltammetry was studied taking into account those conditions which have an influence on the accumulation step (electrolyte, pH, time, potential, drop size and stirring rate), rest time and stripping step (pulse amplitude and scan rate). Oxazepam can be detd. at a hanging mercury drop electrode by differential-pulse voltammetry in 0.008 M Britton-Robinson buffer at pH 2.0 with a -0.50 V accumulation potential. Its detection limit was found to be 3.6 .times. 10-10 M (30-s accumulation) and the relative std. deviation for oxazepam concns. in the range 2.8 .times. 10-8-4.0 .times. 10-7 M is lower than 2.8% (80-s accumulation). In addn., a procedure using adsorptive stripping voltammetry was developed to study the interactions occurring between human albumin and the camazepam metabolic series (camazepam, temazepam and oxazepam). The interactions decreased in the order temazepam > oxazepam > camazepam and the groups and structural modifications favoring interaction were detd.

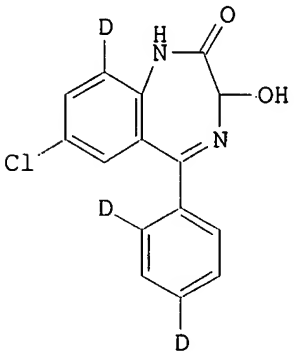
RX(1) OF 1 **A** ===> **B**



A B

RX(1) RCT A **36104-80-0**
PRO B **846-50-4**

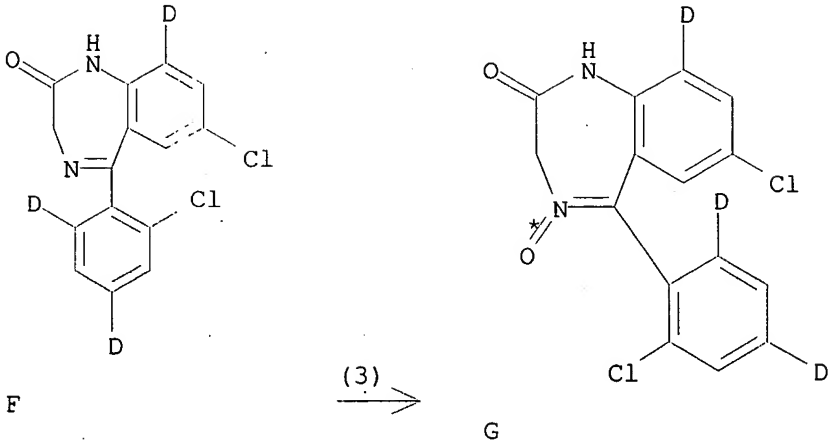
L61 ANSWER 6 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 114:185445 CASREACT
TITLE: Synthesis of deuterium labeled lorazepam
AUTHOR(S): Koves, G. J.
CORPORATE SOURCE: Cent. Forensic Sci., Toronto, ON, M7A 2G8, Can.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1991), 29(1), 15-22
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Synthesis of 2H3-lorazepam I was achieved by modification of literature procedures for the unlabeled drug. The key step in the seven step procedure was the selective exchange of 2-amino-5,2'-dichlorobenzophenone with deuterium in deuterated acids. Purifns. were carried out by preparative HPLC. I is suitable for use as an internal std. in GC-MS-NICI-SIM quant. anal. in forensic case work.

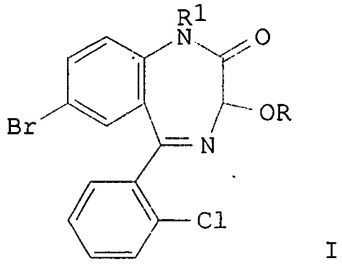
RX(3) OF 21 ...**F** ===> **G**...



F (3) G

RX(3) RCT F **133358-31-3**
PRO G **133358-32-4**
CAT 937-14-4 MCPBA

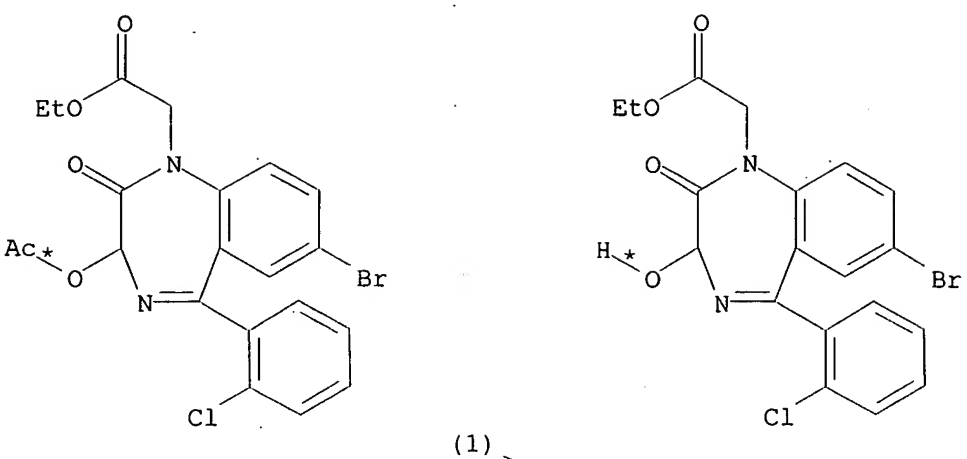
L61 ANSWER 7 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 114:6467 CASREACT
TITLE: Basic hydrolysis of 3-acetoxy-7-bromo-5-(o-chlorophenyl)-1-(ethoxycarbonylmethyl)-1,2-dihydro-3H-1,4-benzodiazepin-2-one
AUTHOR(S): Mazurov, A. A.; Dvorkin, A. A.; Simonov, Yu. A.; Andronati, S. A.
CORPORATE SOURCE: Fiz.-Khim. Inst. im. Bogatskogo, Odessa, 270080, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1990), (5), 685-90
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

AB The ease of selective hydrolysis of title compd. I (R = Ac, R1 = CH2CO2Et) with 1 equiv of base to hydroxy ketone I (R = H, R1 same) was attributed to anchimeric assistance from the ethoxycarbonyl group. Hydrolysis with 2 equiv of base in aq. MeOH afforded the transesterification product I [R = H, R1 = CH2CO2Me (II)]. II crystd. from benzene in the P212121 space group; this guarantees that crystn. is accompanied by autoresoln., forming crystals of a single enantiomer. The crystal and mol. structure of II was detd. by x-ray crystallog.

RX(1) OF 2 **A** ===> **B**

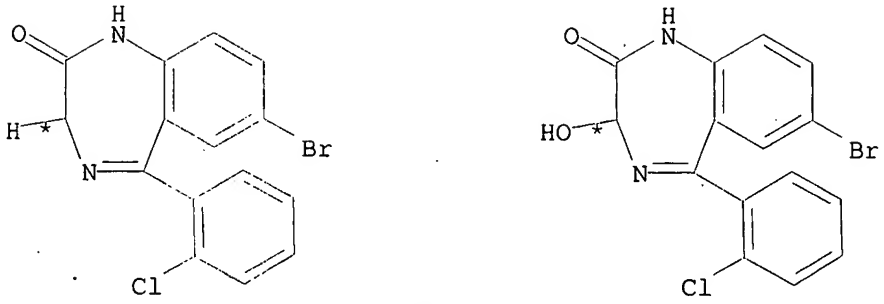


A (1) B
YIELD 78%

RX(1) RCT A **130788-45-3**
RGT C 1310-73-2 NaOH
PRO B **130788-47-5**
SOL 67-56-1 MeOH, 7732-18-5 Water
NTE Reaction products depend on conditions

L61 ANSWER 8 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 113:113735 CASREACT
TITLE: Microbial synthesis of 3-hydroxy derivatives of 1,4-benzodiazepine-2-ones
AUTHOR(S): Davidenko, T. I.; Zabolotskaya, N. N.
CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1990), 24(5), 65-7
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Strains of actinomyces and yeast which effectively accomplish hydroxylation of 1,4-benzodiazepin-2-ones to form optically active compds. were identified. The conditions for their hydroxylation were developed. The hydroxylase system of Saccharomyces cerevisiae was shown to contain cytochrome P 450 and NADPH-cytochrome-C-reductase. It was concluded that the hydroxygenase system of actinomyces had specificity. The prepn. and physicochem. properties of 8 new benzodiazepinones are reported.

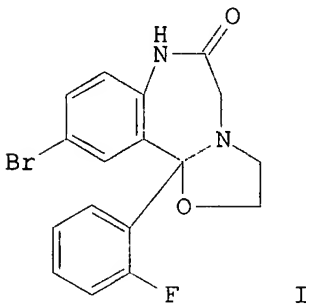
RX(1) OF 8 **A** ===> **B**



A (1) B

RX(1) RCT A **51753-57-2**
PRO B **70030-11-4**

L61 ANSWER 9 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 111:56925 CASREACT
TITLE: Asymmetric transformation. II. Racemization reaction of 1,4-benzodiazepinooxazole derivative
AUTHOR(S): Okada, Yutaka; Takebayashi, Toyonori
CORPORATE SOURCE: Process Dev. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(10), 3787-92
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

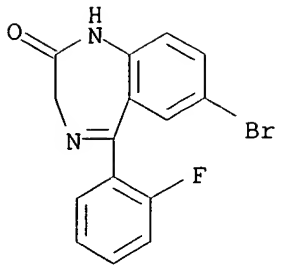


I

uses solvent excluded by proviso

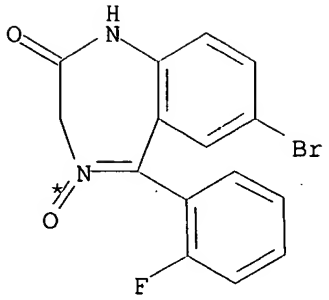
AB Optically active crystals of 10-bromo-11b-(2-fluorophenyl)-2,3,7,11b-tetrahydrooxazolo[3,2-d][1,4]benzodiazepin-6(5H)-one (I) were obtained by preferential crystn.; they were sometimes levorotatory and sometimes dextrorotatory. This phenomenon was an example of second-order asym. transformation between enantiomers. The rapid racemization reaction, essential for asym. transformation, was obsd. in MeOH. The decrease of optical rotation obeyed pseudo first-order kinetics, and the half-lives of the racemization in MeOH were 21 s at 30.degree., 37 s at 20.degree., and 70 s at 10.degree.. The mechanism and factors which affect the rate of the racemization are discussed.

RX(2) OF 7 ...**B** ===> **D**...



B

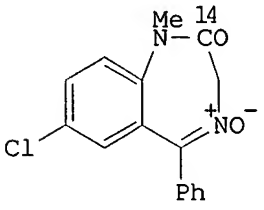
(2) ⟹



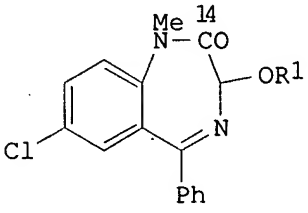
D
YIELD 81%

RX(2) RCT B **2647-50-9**
RGT E 79-21-0 AcOOH
PRO D **10329-38-1**
SOL 75-09-2 CH2Cl2 solvent ~~expld~~ excluded by proviso

L61 ANSWER 10 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 107:217605 CASREACT
TITLE: Synthesis of 7-chloro-1,3,-dihydro-3-hydroxy-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one-2-14C (2-14C-temazepam)
AUTHOR(S): Dain, Jeremy G.
CORPORATE SOURCE: Dep. Drug Metab., Sandoz Res. Inst., East Hanover, NJ, 07936, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(5), 499-504
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



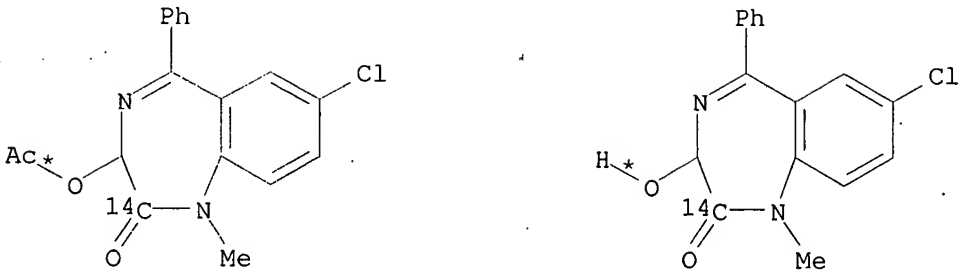
II



III

AB Condensation of ClCH214COCl with 5,2-Cl(RNMe)C6H3Bz (I, R = H) gave amide I (R= 14COCH2Cl). Cyclocondensation of H2NOH and I (R = 14COCH2Cl) gave benzodiazepine oxide II. II was converted to acetate III (R1 = Ac) with Ac2O and hydrolyzed to the title compd. III (R1 = H) in 3.8% overall radiochem. yield.

RX(5) OF 15 ...**M** ===> **O**



M (5) O

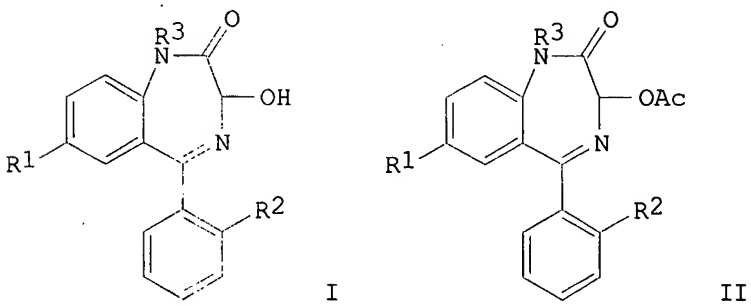
YIELD 23%

RX(5) RCT M **111257-65-9**
RGT P 7664-93-9 H2SO4
PRO O **111257-66-0**
SOL 7664-93-9 H2SO4

L61 ANSWER 11 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 105:191141 CASREACT
TITLE: 3-Hydroxy-1,3-dihydro-2H-1,4-benzodiazepin-2-ones
INVENTOR(S): Andronati, S. A.; Mazurov, A. A.; Dimitrishchuk, G. V.
PATENT ASSIGNEE(S): Physical-Chemical Institute, Academy of Sciences, Ukrainian S.S.R., USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret. 1985, (23), 86. CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 1162800	A1	19850623	SU 1982-3543660	19821213

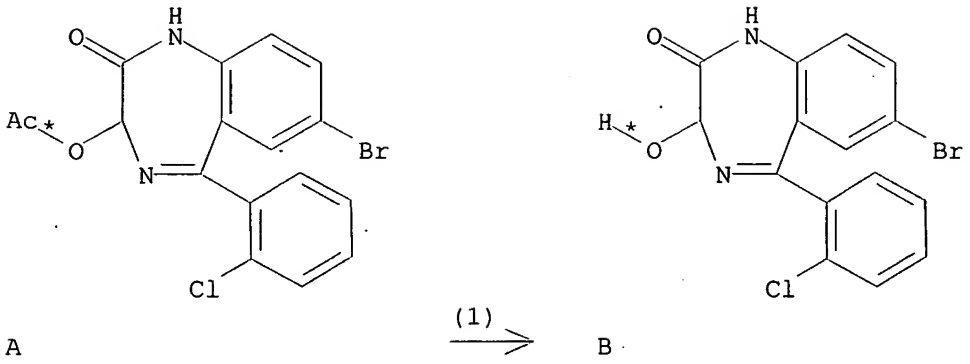
PRIORITY APPLN. INFO.: SU 1982-3543660 19821213
GI



I II

AB The title compds. (I; R1 = H, halo, C1-4 alkyl; R2 = H, halo; R3 = H, C1-4 alkyl) are prepd. by reacting acetoxydihydrobenzodiazepinones II with a deacylating agent. The prepn. of I is accelerated and simplified by using hydrazine hydrate as the deacylating agent, and by conducting the reaction at 40-60.degree. and pH 8-9.

RX(1) OF 1 **A** ===> **B**



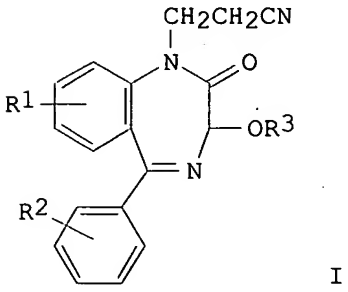
A (1) B

RX(1) RCT A **70030-10-3**
PRO B **70030-11-4**

L61 ANSWER 12 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 104:168499 CASREACT
TITLE: Cyanoethylated 1,4-benzodiazepines
INVENTOR(S): Schlager, Ludwig H.
PATENT ASSIGNEE(S): Gerot-Pharmazeutika G.m.b.H., Austria
SOURCE: Austrian, 5 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 379391	B	19851227	AT 1984-150	19840118
AT 8400150	A	19850515		
ES 539059	A1	19851116	ES 1984-539059	19841226
NO 8500189	A	19850719	NO 1985-189	19850117
NO 161672	B	19890605		
NO 161672	C	19890913		
PRIORITY APPLN. INFO.:			AT 1984-150	19840118

GI

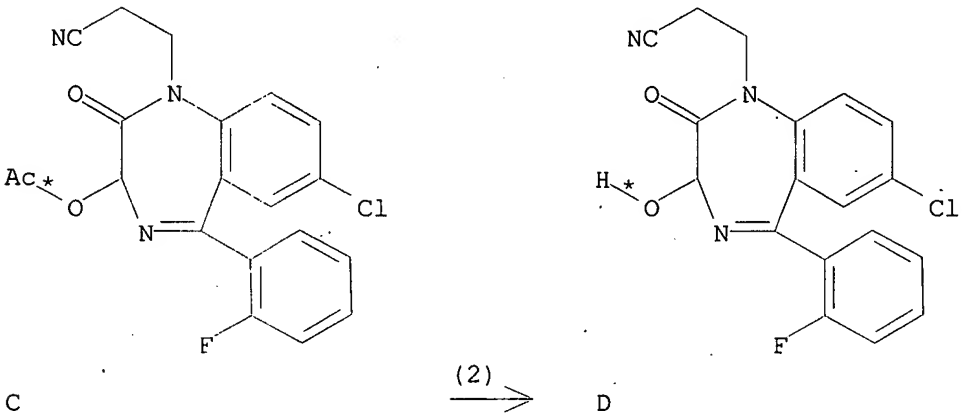


I

AB Soporific (no data) title compds (I: R1 = H, CF3, halo, NO2; R2 = H, halo;

R3 = H) were prepd. Thus, 3-(acetyloxy)-7-chloro-5-(2-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one and CH2:CHCN were stirred at room temp. with a catalytic amt. of PhCH2N+Me3OH- to give 93.7% I (R1 = 7-Cl, R2 = 2-F, R3 = Ac) which was sapond. to give 93% I (R1 = 7-Cl, R2 = 2-F, R3 = H).

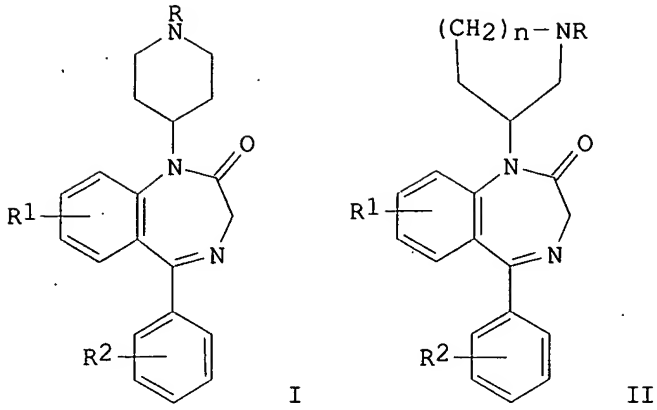
RX(2) OF 3 ...**C** ===> **D**



C D

RX(2) RCT C **101661-96-5**
PRO D **75696-02-5**

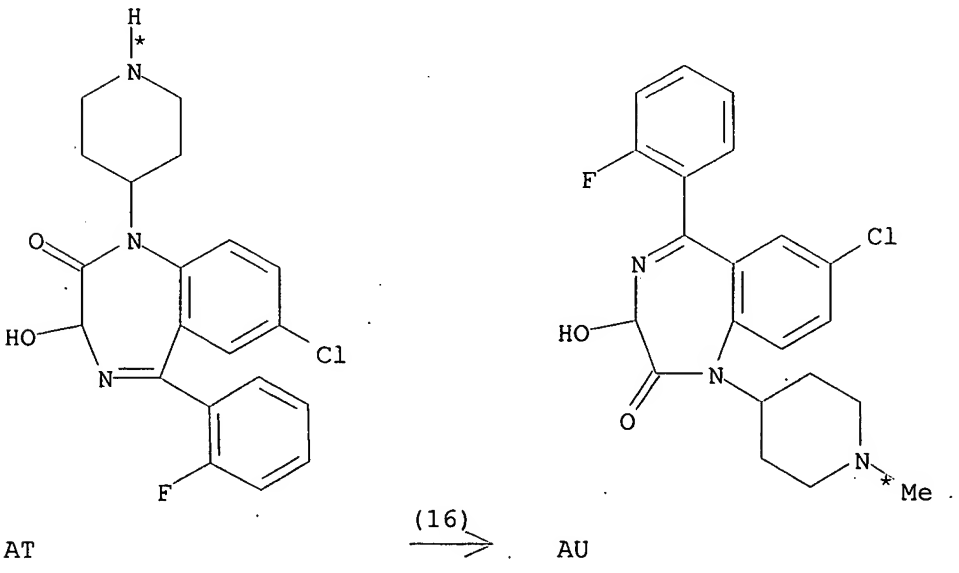
L61 ANSWER 13 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 103:37458 CASREACT
TITLE: 1-Azacycloalkyl-1,4-benzodiazepin-2-ones with antianxiety-antidepressant actions
AUTHOR(S): Sugasawa, Tsutomu; Adachi, Makoto; Sasakura, Kazuyuki; Matsushita, Akira; Eigyo, Masami; Shiomi, Teruo; Shintaku, Haruyuki; Takahara, Yukio; Murata, Shunji
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, 553, Japan
SOURCE: Journal of Medicinal Chemistry (1985), 28(6), 699-707 CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB A series of 1-azacycloalkyl-1,4-benzodiazepin-2-ones I and II (R = H, Me, PhCH2CH2; R1, R2 = H, halo; n = 1, 2) were synthesized from 1-azacycloalkyl-2-benzoylanilines and corresponding imines and then evaluated for their central nervous system activities. Pharmacol. data showed that some of these compds. have potent antidepressant properties, as assessed by their antagonism of tetrabenzine induced ptosis and their inhibition of [3H]norepinephrine uptake into rat brain synaptosomes, as well as their moderate antianxiety properties of preventing of pentylenetetrazol convulsion, suppressing conflict behavior, and displacing potential for [3H]diazepam binding. Secondary function of the azacyclic ring at position 1 was essential for the prodn. of the antidepressant properties. Of these new series, I (R = H; R1 = R2 = F) has the potential to become a useful antidepressant drug with a moderate antianxiety property.

RX(16) OF 407 ...**AT** ===> **AU**...

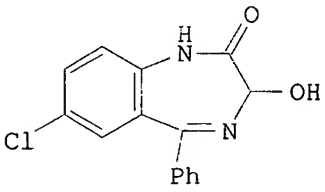


AT (16) AU

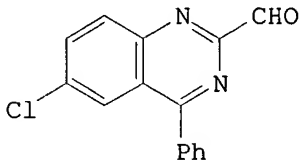
RX(16) RCT AT **96110-74-6**
RGT AV 77-78-1 Me2SO4, AW 584-08-7 K2CO3
PRO AU **96110-75-7**

SOL 75-05-8 MeCN

L61 ANSWER 14 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 102:166099 CASREACT
TITLE: Quantitative [1,3,2,3]-elimination of water from oxazepam
AUTHOR(S): Kaupp, Gerd; Knichala, Bernd
CORPORATE SOURCE: Fachber. Chem.-Org. Chem., Univ. Oldenburg, Oldenburg, D-2900, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1985), 118(2), 462-7
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



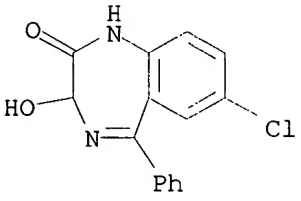
I



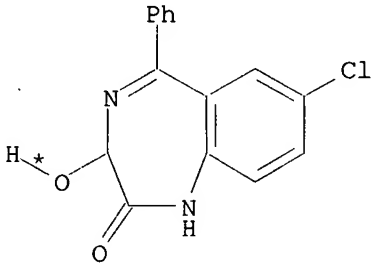
II

AB D-labeling expts. indicated that in the pyrolysis of oxazepam (I) at 150.degree. to give aldehyde II the H attached to C-3 in I becomes the formyl H in II. The mechanism is discussed. The O-Ac deriv. of I decomps. nonselectively at higher temps. with no II being detectable.

RX(2) OF 9 2 **A** ===> **D** + E...

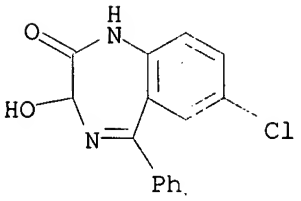


A

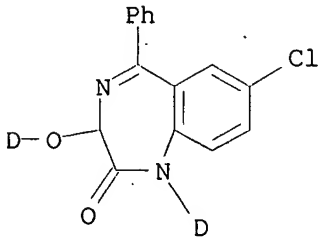


A

(2) →



D

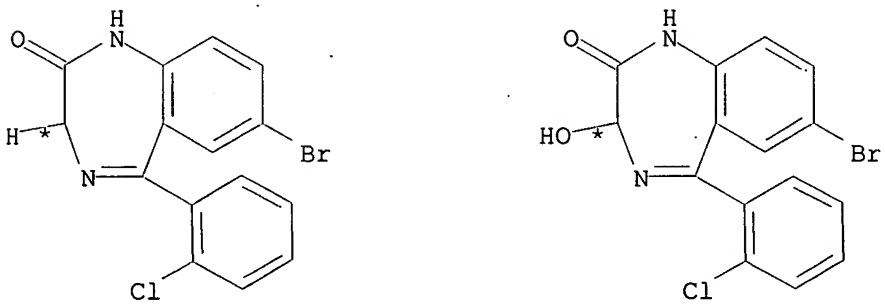


E

RX(2) RCT A **604-75-1**
RGT F 7789-20-0 D2O
PRO D **95926-86-6**, E 95926-87-7
SOL 75-05-8 MeCN

L61 ANSWER 15 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 102:147424 CASREACT
TITLE: Hydroxylation of 1,4-benzodiazepin-2-ones by actinomycetes
AUTHOR(S): Davidenko, T. I.; Zabolotskaya, N. N.; Milienko, N. P.; Andronati, S. A.; Kuznetsov, V. D.; Bogatskii, A. V.
CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, USSR
SOURCE: Doklady Akademii Nauk SSSR (1984), 278(4), 878-81 [Chem.]
CODEN: DANKAS; ISSN: 0002-3264
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Twenty-four strains of actinomycetes were able to transform 6 title compds. to the corresponding 3-hydroxy-1,4-benzodiazepin-2-ones. The highest rate of hydroxylation was obsd. with Actinomyces roseochromogenes, A. lavendulae, and Streptomyces viridis. The yield of 3-hydroxy derivs. was 30-40%. When the actinomycetes were immobilized in various carriers, esp. carrageenan [9000-07-1], 65% of the hydroxylation activity was retained. The 3-hydroxy derivs. are used as tranquilizers.

RX(1) OF 12 **A** ===> **B**



A B
YIELD 30%

RX(1) RCT A **51753-57-2**
PRO B **70030-11-4**

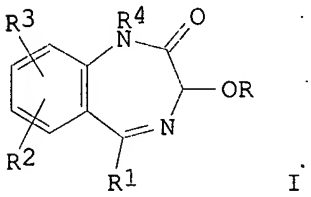
L61 ANSWER 16 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 100:51612 CASREACT
TITLE: 3-Hydroxybenzodiazepinones
INVENTOR(S): Hardtmann, Goetz Eduard; Repic, Oljan; Vogt, Susi
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3314893	A1	19831103	DE 1983-3314893	19830425
US 4412952	A	19831101	US 1982-373450	19820430
FR 2526021	A1	19831104	FR 1983-6804	19830422
FR 2526021	B1	19870612		
CH 655930	A	19860530	CH 1983-2176	19830422
GB 2120245	A1	19831130	GB 1983-11446	19830427
GB 2120245	B2	19851023		
JP 58194865	A2	19831112	JP 1983-74194	19830428
CA 1195326	A1	19851015	CA 1983-426924	19830428

PRIORITY APPLN. INFO.: US 1982-373450 19820430

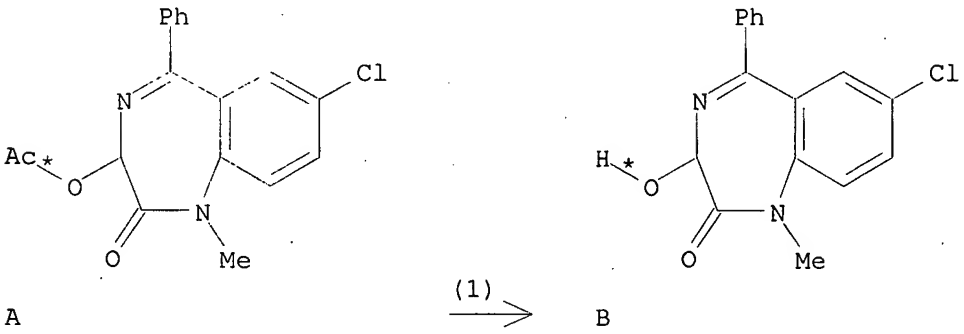
GI



I

AB Hydroxybenzodiazepinones I [R = H; R1 = (un)substituted Ph; R2, R3 = H, F3C, MeSO2, Br, Cl, NO2, R4 = alkyl] were prepd. in high yield and purity by sapon. of I (R = acyl) with KOR5 (R5 = H, alkyl) in alc. Thus, I (R = Ac, R1 = Ph, R2 = 7-Cl, R3 = H, R4 = Me) was refluxed in MeOH with KOH to give, after crystn. from EtOH, 82.9% I (R = H, R1 = Ph, R2 = 7-Cl, R4 = Me) of 99.8% purity.

RX(1) OF 1 **A** ===> **B**



A B

RX(1) RCT A **18818-64-9**
PRO B **846-50-4**

L61 ANSWER 17 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 96:160848 CASREACT
TITLE: 3-Hydroxy-7-bromo-5-(o-, m-, p-chloro) phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one and 3-hydroxy-3-methyl-7-bromo-5-(o-, m-, p-chloro) phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one by fermentation

Searched by Barb O'Bryen, STIC 308-4291

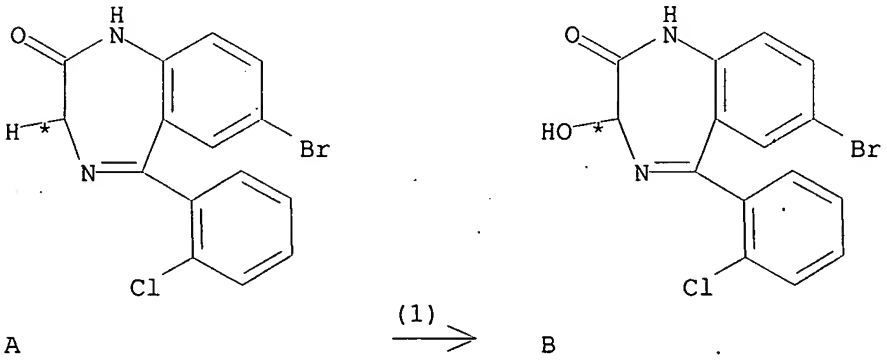
INVENTOR(S): Bogatskii, A. V.; Kuznetsov, V. D.; Davidenko, T. I.; Zabolotskaya, N. N.; Sereda, N. P.; Andronati, S. A.; Yakubovskaya, L. N.
PATENT ASSIGNEE(S): Institute of Physical Chemistry, Academy of Sciences, Ukrainian S.S.R., USSR; Institute of Microbiology
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1981, (45), 144.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 887625	A1	19811207	SU 1980-2928358	19800208

PRIORITY APPLN. INFO.: SU 1980-2928358 19800208

AB The title compds. are obtained by cultivating Streptoverticillium cinnamoneum VKM A-609 or Streptomyces viridis VKM A-607 in a nutrient medium contg. corn ext. 1.0, glucose 0.5, NaCl 0.5, (NH4)2SO4 0.3, CaCO3 0.5 and starch 1.5 g/100 g H2O at pH 6.8-7.0, adding (3-12 mg/100 mg medium) 7-bromo-5-(o-, m-, or p-chloro)phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-one, incubating for 2-5 days at 28.degree., sepg. the products by extn. with CHCl3, EtOAc, petroleum ether, or a mixt. of C2H4Cl2 and EtOAc, and purifying by recrystn. from alc. or by column chromatog. on Al2O3, eluting with a mixt. of MeOH or EtOH and HOAc.

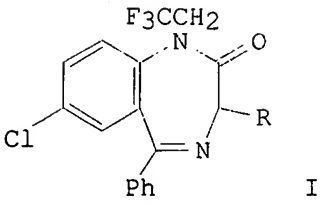
RX(1) OF 1 **A** ===> **B**



A B

RX(1) RCT A **51753-57-2**
PRO B **70030-11-4**

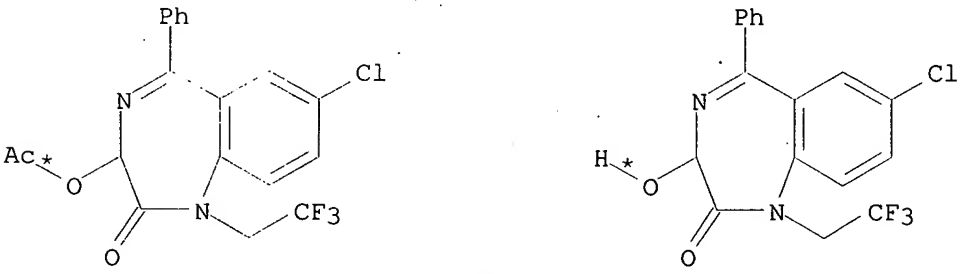
L61 ANSWER 18 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 94:121481 CASREACT
TITLE: New synthesis of 2-(2',2',2'-trifluoroethyl)-amino-5-chlorobenzophenone and related studies
AUTHOR(S): Oklobdzija, Milan; Fajdiga, Tatjana; Kovac, Tomislav; Zonno, Franco; Sega, Alessandro; Sunjic, Vitomir
CORPORATE SOURCE: Chem. Res. Co., San Giovanni al Natisone, Italy
SOURCE: Acta Pharmaceutica Jugoslavica (1980), 30(3), 121-33
CODEN: APJUA8; ISSN: 0001-6667
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The haloazepam (I, R = H) intermediate 2,4-BzClC6H3NHCH2CF3 (II) was prepd. by trifluoroacetylating 2,4-BzClC6H3NH2, redn. of 2,4-BzClC6H3NHCOCF3 with NaAlH2Et2, and oxidn. of 2,4-HOCHPhClC6H3NHCH2CF3 with pyridinium dichromate. II was also obtained by treating 2,4-BzClC6H3NH2 with CF3CO2H-NaBH4. Acylation of II with BrCH2COBr and ring closure with hexamine gave I (R = H) which was acetoxylated and treated with NaOMe to give I (R = OH). Reductive trifluoroethylation of demethyldiazepam occurred in the 4-position only.

RX(18) OF 53 ...**X** ===> **AA**



X AA

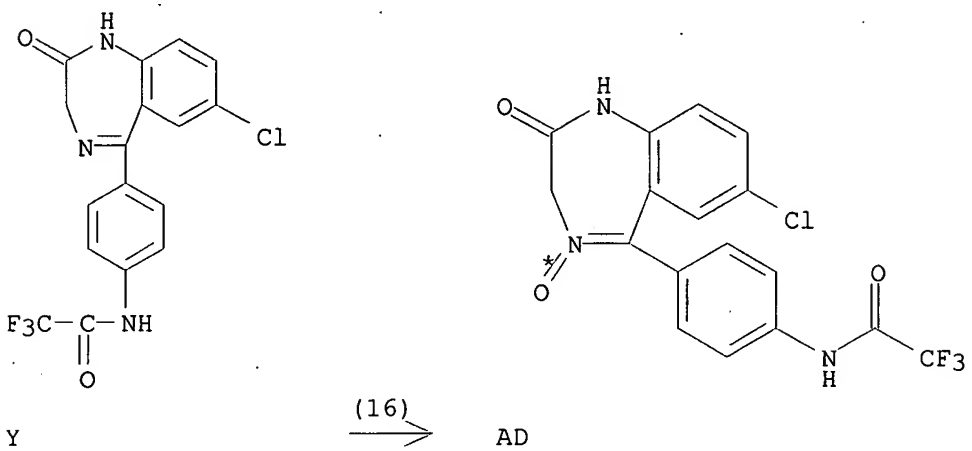
RX(18) RCT X **22753-74-8**
PRO AA **22753-75-9**
CAT 124-41-4 NaOMe

L61 ANSWER 19 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 92:41904 CASREACT
TITLE: Quinazolines and 1,4-benzodiazepines. LXXXIX: Haptens useful in benzodiazepine immunoassay development
AUTHOR(S): Earley, James V.; Fryer, R. Ian; Ning, Robert Y.
CORPORATE SOURCE: Dep. Chem. Res., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Journal of Pharmaceutical Sciences (1979), 68(7), 845-50
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Benzodiazepines I (R = H, Me; R1 = H, AcO, HO; R2 = HO, F3CCONH, MeO2CCH2O, MeO, H2NCOCH2O, H2NNHCOCH2O, H2N; R3 = H, H2NC6H4N:N; n = 1, 0), II (R4 = HO, H2N, MeO2CCH2O, H2NNHCOCH2O, H2NCH2CH2CH2O), and III (R5 = H, HO2CCH2CH2O; R6 = HN, NO2; R7 = H, Cl) were prepd. as haptens for use in immunoassay anal. Thus, cyclocondensation of the benzophenone IV in NH3(l) gave 67% I (R = R1 = R3 = H; R2 = HO; n = 0), and treatment of quinazoline V with MeNH2 in MeOH gave II (R4 = HO).

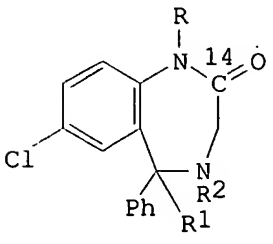
RX(16) OF 123 ...**Y** ===> **AD**...



Y (16) AD

RX(16) RCT Y **67445-91-4**
PRO AD **67445-92-5**
CAT 937-14-4 MCPBA

L61 ANSWER 20 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 92:22479 CASREACT
TITLE: Synthesis of 2-14C-labeled 3H-1,4-benzodiazepines
AUTHOR(S): Tegyey, Zsuzsanna; Maksay, G.; Otvos, L.
CORPORATE SOURCE: Cent. Res. Inst. Chem., Budapest, Hung.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1979), 16(3), 377-85
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

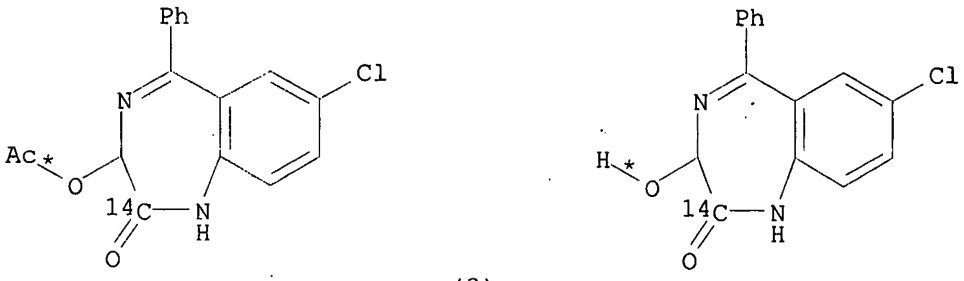


I

AB Di- and tetrahydrobenzodiazepinones I (R = H, R1R2 = bond; R = Me, R1 = H, R2 = H, CONH2) were prepd. (radiochem. yield 28.9, 9.5 and 25.3%, resp.)

in 5, 3 and 4 steps, resp., from PhCH2O2CNHCH214COCl and 4,2-Cl(PhCO)C6H3NHR.

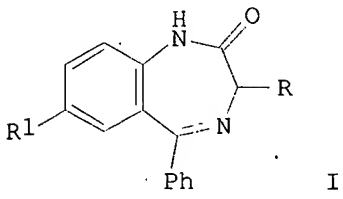
RX(3) OF 14 ...**G** ===> **H**



G (3) H
YIELD 79%

RX(3) RCT G **72216-21-8**
PRO H **3855-66-1**

L61 ANSWER 21 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 91:157698 CASREACT
TITLE: 1,4-Benzodiazepines and their cyclic homologs and analogs. 30. Synthesis and properties of 3- and 7-amino-5-phenyl-1,2-dihydro-3H-1,4-benzodiazepin-2-ones
AUTHOR(S): Zhilina, Z. I.; Bogatskii, A. V.; Andronati, S. A.; Danilina, N. I.
CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, 270080, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1979), (4), 545-9
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

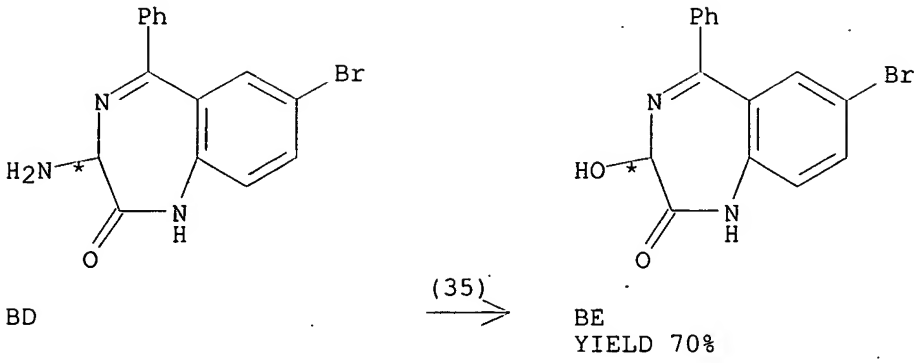


I

AB The 3-aminobenzodiazepinones I (R = NH2; R1 = H, Me, Br, Cl) (II) were prepd. from 2,4-(Bz)R1C6H3NHCOCH2Cl by iodination to give 2,4-(Bz)R1C6H3NHCOCH2I, which underwent hydroxyamination to give 2,4-(Bz)R1C6H3NHCOCH2NHOH; treatment of the latter with Ac2O and then cyclocondensation in EtOH contg. NH3 and hydrolysis gave II. 7-Aminobenzodiazepinone I (R = H; R1 = NH2) (III) was prepd. by redn. of I (R1 = NO2). II and III formed Schiff bases on condensation with benzaldehydes in aprotic solvents contg. acid catalysts, e.g. ZnCl2. Treatment of I (R = AcNH; R1 = Cl) with P2S5 gave I [R = MeC(S)NH; R1 = Cl], and diazotization-hydrolysis of I (R = NH2; R1 = Br) gave I (R = HO).

Polarog. redn. curves of the Schiff bases of II were detd.

RX(35) OF 146 ...**BD** ===> **BE**

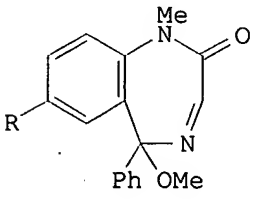


BD

BE
YIELD 70%

RX(35) RCT BD **70890-49-2**
RGT BF 7782-77-6 HNO2
PRO BE **37891-18-2**

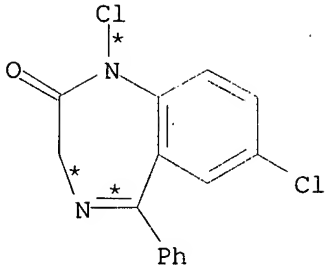
L61 ANSWER 22 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 87:33437 CASREACT
TITLE: 5-Aryl-1,5-dihydro-2H-1,4-benzodiazepin-2-one derivatives as antianxiety agents
AUTHOR(S): Ogata, Masaru; Matsumoto, Hiroshi; Hirose, Katsumi
CORPORATE SOURCE: Shionogi Res. Lab., Shionogi and Co., Ltd., Osaka, Japan
SOURCE: Journal of Medicinal Chemistry (1977), 20(6), 776-81
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



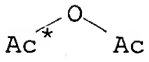
I, R=Cl
II, R=NO_2

AB A series of 18 7-chloro- or 7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one derivs. were prepd. and tested in mice for acute toxicity and activity as muscle relaxants, tranquilizers, and anticonvulsants. 7-Chloro-1,5-dihydro-5-methoxy-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one (I) [62658-15-5] and 1,5-dihydro-5-methoxy-1-methyl-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one (II) [62159-90-4] had activity comparable to or greater than diazepam [439-14-5]. Structure-activity relations are discussed.

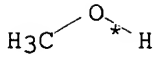
RX(93) OF 101 COMPOSED OF RX(8), RX(9), RX(12), RX(15), RX(6)
RX(93) **B** + E + I ===> **Q**



B

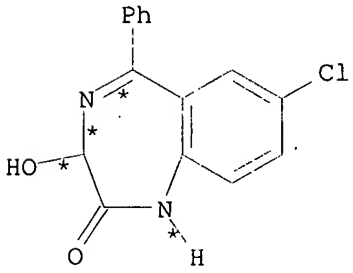


E



I

5 STEPS



Q
YIELD 81%

RX(8) RCT B **10378-81-1**, E 108-24-7
RGT G 7697-37-2 HNO3
PRO T 62658-06-4

RX(9) RCT T 62658-06-4
PRO U 62658-09-7
CAT 74-89-5 MeNH2

RX(12) RCT U 62658-09-7, I 67-56-1
PRO N 62159-89-1
SOL 67-56-1 MeOH

RX(15) RCT N 62159-89-1
PRO K 61983-99-1
CAT 121-44-8 Et3N

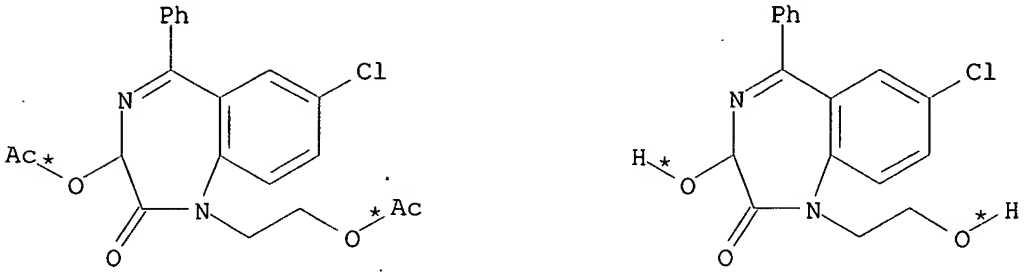
RX(6) RCT K 61983-99-1
PRO Q **604-75-1**

L61 ANSWER 23 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 83:164140 CASREACT
TITLE: New series of benzodiazepines. 1-Hydroxyalkyl derivatives of 1,3-dihydro-2H-1,4-benzodiazepin-2-ones
AUTHOR(S): Tamagnone, G. F.; De Maria, R.; De Marchi, F.
CORPORATE SOURCE: Res. Dep., Schiapparelli S.p.A., Turin, Italy
SOURCE: Arzneimittel-Forschung (1975), 25(5), 720-2
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English

Searched by Barb O'Bryen, STIC 308-4291

GI For diagram(s), see printed CA Issue.
AB Twenty-four potential hypnotics I [R = OH, O2C(CH2)2CO2H), OAc, Cl, NEt2; R1 = H, OAc, OH, OEt; R2 = H, Cl, F; R3 = Cl, NO2, n = 2, 3] or their oxides were prepd. by 1-alkylating the appropriate phenylbenzodiazepinones and usual reactions (acylation, hydrolysis, etc.).

RX(3) OF 22 **F** ===> **G**...

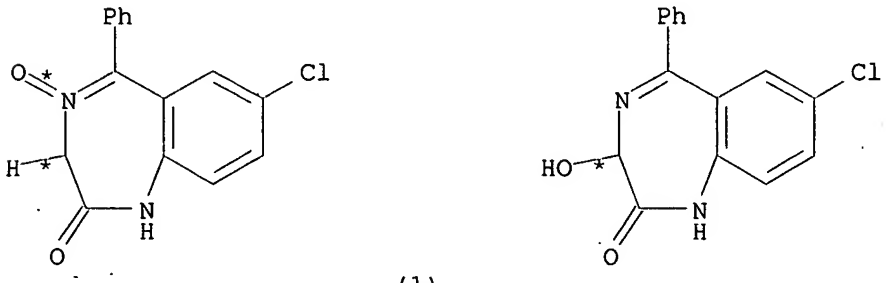


F (3) G
YIELD 85%

RX(3) RCT F **56875-82-2**
RGT H 7664-41-7 NH3
PRO G **51230-34-3**

L61 ANSWER 24 OF 24 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 74:31735 CASREACT
TITLE: Nitrone isomerization in the 1,4-benzodiazepine series
AUTHOR(S): Schlager, Ludwig H.
CORPORATE SOURCE: Gerot Pharm., Vienna, Austria
SOURCE: Tetrahedron Letters (1970), (51), 4519-20
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The nitrone (I) is converted to oxazepam (II) in a 1-step reaction by treatment with a Lewis acid in the presence of a nitrile, such as MeCN or acrylonitrile. I is treated with BF3 to give an adduct which is kept in the nitrile at room temp. to give II. II is obtained from I without adduct formation when AlCl3 is used.

RX(1) OF 1 **A** ===> **B**



A (1) B

RX(1) RCT A **963-39-3**
RGT C 7446-70-0 AlCl3
PRO B **604-75-1**
SOL 109-99-9 THF, 75-05-8 MeCN
NTE Classification: N-Deoxygenation; Hydroxylation; Migration; # Conditions: AlCl3; THF; MeCN; 20 deg; # Comments: acrylonitrile can also be used as solvent,BF3.Et2O as alternative reagent

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